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 SDIs in CAPlus
 NEWS 9 May 27 CAPlus super roles and document types searchable in REGISTRY
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 NEWS 11 Jun 22 STN Patent Forums to be held July 19-22, 2004

NEWS EXPRESS MARCH 31 CURRENT WINDOWS VERSION IS V7.00A, CURRENT
 MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP),
 AND CURRENT DISCOVER FILE IS DATED 26 APRIL 2004

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* * * * * STN Columbus * * * * *

FILE 'HOME' ENTERED AT 19:21:10 ON 22 JUN 2004

=> file reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.21	0.21

FILE 'REGISTRY' ENTERED AT 19:21:16 ON 22 JUN 2004

USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.

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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 21 JUN 2004 HIGHEST RN 697224-75-2

DICTIONARY FILE UPDATES: 21 JUN 2004 HIGHEST RN 697224-75-2

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2004

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:

<http://www.cas.org/ONLINE/DBSS/registryss.html>

=>

L1 STRUCTURE UPLOADED

=> d l1

L1 HAS NO ANSWERS

L1 STR

=> s l1

SAMPLE SEARCH INITIATED 19:21:50 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 8863 TO ITERATE

11.3% PROCESSED 1000 ITERATIONS

4 ANSWERS

INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS: 171619 TO 182901

PROJECTED ANSWERS: 352 TO 1066

L2 4 SEA SSS SAM L1

=> s l1 full

THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 155.00 U.S. DOLLARS

DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y

FULL SEARCH INITIATED 19:21:54 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 175967 TO ITERATE

100.0% PROCESSED 175967 ITERATIONS

579 ANSWERS

SEARCH TIME: 00.00.07

L3 579 SEA SSS FUL L1

=> file hcaplus

COST IN U.S. DOLLARS

SINCE FILE TOTAL

ENTRY SESSION

FULL ESTIMATED COST

155.42 155.63

FILE 'HCAPLUS' ENTERED AT 19:22:04 ON 22 JUN 2004

USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.

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FILE COVERS 1907 - 22 Jun 2004 VOL 140 ISS 26
 FILE LAST UPDATED: 21 Jun 2004 (20040621/ED)

This file contains CAS Registry Numbers for easy and accurate
 substance identification.

=> s l3/thu

108 L3
 600602 THU/RL
 L4 39 L3/THU
 (L3 (L) THU/RL)

=> s l4 and arthritis?

32853 ARTHRITIS?
 L5 6 L4 AND ARTHRITIS?

=> s l5 and faull, a?/au

34 FAULL, A?/AU
 L6 1 L5 AND FAULL, A?/AU

=> d l6, ibib abs fhitr, 1

L6 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text	Citing References
ACCESSION NUMBER:	1999:126819 HCAPLUS
DOCUMENT NUMBER:	130:182354
TITLE:	Preparation of substituted indoles for treatment of a disease or condition mediated by monocyte chemoattractant protein-1 (MCP-1)
INVENTOR(S):	Barker, Andrew John; Kettle, Jason Grant; Faull, Alan Wellington
PATENT ASSIGNEE(S):	Zeneca Limited, UK
SOURCE:	PCT Int. Appl., 64 pp. CODEN: PIXXD2
DOCUMENT TYPE:	Patent
LANGUAGE:	English
FAMILY ACC. NUM. COUNT:	1
<u>PATENT INFORMATION:</u>	

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9907351	A2	19990218	WO 1998-GB2341	19980804
WO 9907351	A3	19990514		
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, HR, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
AU 9886381	A1	19990301	AU 1998-86381	19980804
AU 745907	B2	20020411		
EP 1003504	A2	20000531	EP 1998-937659	19980804
EP 1003504	B1	20030702		
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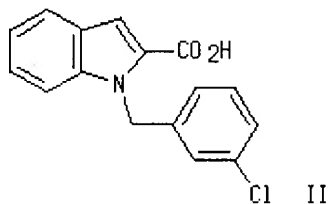
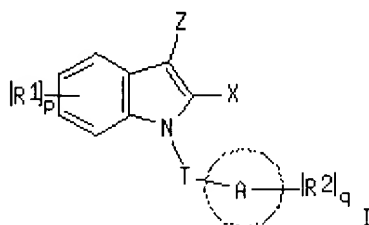
BR 9811818	A	20000815	BR 1998-11818	19980804
TR 200000289	T2	20000821	TR 2000-200000289	19980804
JP 2001513494	T2	20010904	JP 2000-506944	19980804
RU 2217142	C2	20031127	RU 2000-105901	19980804
PT 1003504	T	20031128	PT 1998-937659	19980804
ZA 9807090	A	19990208	ZA 1998-7090	19980806
HR 2000000061	A1	20001231	HR 2000-61	20000203
US 6441004	B1	20020827	US 2000-485061	20000203
NO 2000000573	A	20000204	NO 2000-573	20000204
HK 1027979	A1	20031031	HK 2000-107435	20001121
US 2003119830	A1	20030626	US 2002-194969	20020715

PRIORITY APPLN. INFO.:

GB 1997-16657	A	19970807
WO 1998-GB2341	W	19980804
US 2000-485061	A1	20000203

OTHER SOURCE(S):
GI

MARPAT 130:182354



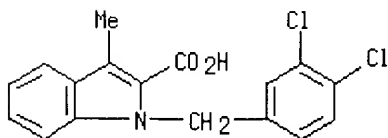
AB The title compds. [I; R1 = CF3, alkyl, halo, etc.; p = 0-4; T = (CHR4)m (wherein R4 = H, alkyl; m = 1-3); X = CO2R4, SO3H, CN, etc.; A = Ph, naphthyl, furyl, etc.; R2 = CF3, alkyl, halo, etc.; q = 0-4; Z = H, halo, Me, etc.] and their pharmaceutically acceptable salts or in vivo hydrolysable esters, useful in the treatment of a disease or condition mediated by monocyte chemoattractant protein-1 (MCP-1) such as rheumatoid arthritis, asthma, atherosclerosis, psoriasis, inflammatory bowel disease and stroke, were prepd. and formulated. Thus, hydrolysis of Et N-(3-chlorobenzyl)indole-2-carboxylate with 2N NaOH in THF/MeOH afforded 82% II. The tested compds. I showed generally IC50 of < 50 µM in the hMCP-1 receptor binding assay.

IT **220678-49-9P**

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); **THU (Therapeutic use)**; BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of substituted indoles for treatment of a disease or condition mediated by monocyte chemoattractant protein-1 (MCP-1))

RN 220678-49-9 HCAPLUS

CN 1H-Indole-2-carboxylic acid, 1-[(3,4-dichlorophenyl)methyl]-3-methyl-
(9CI) (CA INDEX NAME)



=> d his

(FILE 'HOME' ENTERED AT 19:21:10 ON 22 JUN 2004)

FILE 'REGISTRY' ENTERED AT 19:21:16 ON 22 JUN 2004

L1 STRUCTURE UPLOADED
 L2 4 S L1
 L3 579 S L1 FULL

FILE 'HCAPLUS' ENTERED AT 19:22:04 ON 22 JUN 2004

L4 39 S L3/THU
 L5 6 S L4 AND ARTHRITIS?
 L6 1 S L5 AND FAULL, A?/AU

=> s 15 not 16

L7 5 L5 NOT L6

=> d 17, ibib abs fhitrstr, 1-5

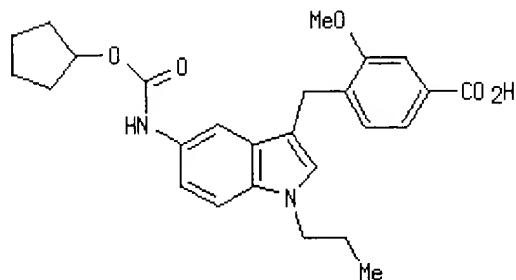
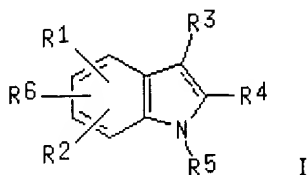
L7 ANSWER 1 OF 5 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text	Citing References
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ACCESSION NUMBER: 2003:1275 HCAPLUS
 DOCUMENT NUMBER: 138:55866
 TITLE: Preparation of indole derivatives as phospholipase
 enzyme inhibitors for treatment of inflammatory
 conditions
 INVENTOR(S): Seehra, Jasbir S.; McKew, John C.; Lovering, Frank;
 Bemis, Jean E.; Xiang, Yibin; Chen, Lihren; Knopf,
 John L.
 PATENT ASSIGNEE(S): Genetics Institute, LLC, USA
 SOURCE: U.S., 57 pp., Cont.-in-part of U. S. Ser. No. 256,062,
 abandoned.
 CODEN: USXXAM
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 6500853	B1	20021231	US 2000-686616	20001011
PRIORITY APPLN. INFO.:			US 1998-113674P	P 19980228
			US 1999-256062	B2 19990224
OTHER SOURCE(S):		MARPAT 138:55866		
GI				

Out good



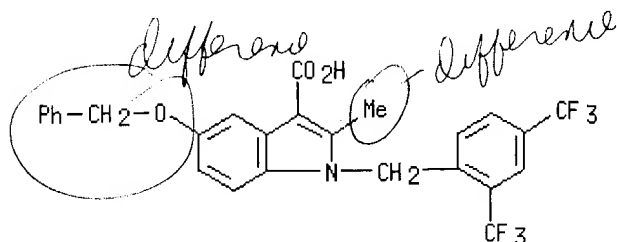
NO

AB Title compds. I [wherein R1 and R6 = independently H, halo, CF₃, alkyl, alkylthio, alkoxy, CN, NO₂, NH₂, Ph, OPh, SPh, CH₂Ph, OCH₂Ph, SCH₂Ph, or (un)substituted amido, carbamido, sulfonyl, etc.; R2 = H, halo, CF₃, OH, alkyl, alkoxy, CHO, CN, NO₂, (un)substituted amino, or alkylsulfonyl; R3 = CO₂H, OPO₃H₂, SO₃H, etc.; R4 = H, CF₃, alkyl, alkoxy, (alkyl)cycloalkyl, CHO, halo, etc.; R5 = alkyl, alkoxy, (alkyl)cycloalkyl, etc.; and pharmaceutically acceptable salts thereof] were prepd. as phospholipase enzyme inhibitors. For example, 5-nitroindole was C3-alkylated (55%) with Me 4-(bromomethyl)-3-methoxybenzoate in dioxane, N-alkylated (57%) with 1-iodopropane in a soln. of THF and NaH, and converted to the amine (80%) by hydrogenation using Pt/C. The amine was converted to the carbamate (39%) by addn. of cyclopentyl chloroformate in CH₂Cl₂ and 4-methylmorpholine, and the resultant ester was hydrolyzed to yield II (71%). The latter inhibited cytosolic phospholipase A₂ (cPLA₂) by 50% at a concn. of 170 μM in a coumarin assay and reduced footpad vol. by 16.61% at a dose of 5 mg/Kg IV in a carrageenan-induced footpad edema test on rats. Thus, I are useful for treatment of inflammatory conditions, such as **arthritis**, inflammatory bowel disease, and asthma (no data).

IT **241497-82-5P**, 1H-Indole-3-carboxylic acid, 1-[[2,4-bis(trifluoromethyl)phenyl)methyl]-2-methyl-5-(phenylmethoxy) -
 RL: PAC (Pharmacological activity); RCT (Reactant); **THU (Therapeutic use)**; **THU (Therapeutic use)**; BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
 (phospholipase inhibitor; prepn. of indole derivs. as phospholipase enzyme inhibitors for treatment of inflammatory conditions)

RN **241497-82-5** HCAPLUS

CN 1H-Indole-3-carboxylic acid, 1-[[2,4-bis(trifluoromethyl)phenyl)methyl]-2-methyl-5-(phenylmethoxy) - (9CI) (CA INDEX NAME)



REFERENCE COUNT:

83

THERE ARE 83 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 2 OF 5 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text	Citing References
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ACCESSION NUMBER: 2002:964145 HCAPLUS
 DOCUMENT NUMBER: 138:19491
 TITLE: A method for treating inflammatory diseases by administering a PPAR- δ agonist
 INVENTOR(S): Forrest, Michael J.; Berger, Joel P.; Moller, David E.; Wright, Samuel
 PATENT ASSIGNEE(S): Merck & Co., Inc., USA
 SOURCE: PCT Int. Appl., 33 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002100351	A2	20021219	WO 2002-US20974	20020607
WO 2002100351	A3	20030501		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
EP 1399151	A2	20040324	EP 2002-746824	20020607
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				

PRIORITY APPLN. INFO.:
 US 2001-297356P P 20010611
 WO 2002-US20974 W 20020607

AB A method for treating, controlling, preventing or reducing the risk of contracting an inflammatory disease or condition in a mammalian patient, comprises (1) selecting a patient in need thereof, and (2) treating the patient with a therapeutically effective amt. of a compn. comprising a PPAR- δ agonist. Inflammatory diseases that may be treated by this method include but are not limited to rheumatoid **arthritis**, juvenile rheumatoid **arthritis**, systemic lupus erythematosus, osteoarthritis, degenerative joint disease, one or more connective tissue diseases, ankylosing spondylitis, and bursitis.

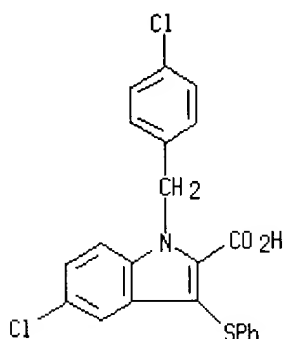
IT **118414-59-8**

RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(PPAR- δ agonist for treating inflammatory disease, and use with other agents)

RN **118414-59-8** HCAPLUS

CN 1H-Indole-2-carboxylic acid, 5-chloro-1-[(4-chlorophenyl)methyl]-3-(phenylthio)- (9CI) (CA INDEX NAME)

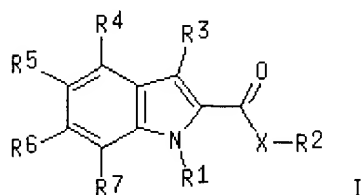


L7 ANSWER 3 OF 5 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text	Citing References
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ACCESSION NUMBER: 2002:293620 HCAPLUS
 DOCUMENT NUMBER: 136:309846
 TITLE: Preparation of substituted indoles as PPAR- γ binding agents
 INVENTOR(S): Stolle, Andreas; Dumas, Jacques P.; Carley, William; Coish, Phillip D. G.; Magnuson, Steven R.; Wang, Yamin; Nagarathnam, Dhanapalan; Lowe, Derek B.; Su, Ning; Bullock, William H.; Campbell, Ann-Marie; Qi, Ning; Baryza, Jeremy L.; Cook, James H.
 PATENT ASSIGNEE(S): Bayer Corporation, USA
 SOURCE: PCT Int. Appl., 233 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002030895	A1	20020418	WO 2001-US42644	20011009
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2002011901	A5	20020422	AU 2002-11901	20011009
US 2003087902	A1	20030508	US 2001-974319	20011009
EP 1341761	A1	20030910	EP 2001-979996	20011009
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
NO 2003001619	A	20030602	NO 2003-1619	20030409
PRIORITY APPLN. INFO.:			US 2000-239195P	P 20001010
			US 2000-243665P	P 20001027
			WO 2001-US42644	W 20011009
OTHER SOURCE(S):			MARPAT 136:309846	
GI				



AB The title compds. [I; R1 = R8R9; R8 = alkyl, alkenyl, alkynyl, etc.; R9 = (un)substituted Ph, cycloalkyl, heterocycloalkyl, etc.; X = (un)substituted NH, S, O; R2 = H, alkyl, halo, alkyl, etc.; R3 = R12R13; R12 = alkyl, alkenyl, alkynyl, CO; R13 = (un)substituted cycloalkyl, cycloalkenyl, heterocycloalkyl, etc.; R4-R7 = H, OH, etc.], useful in treating or preventing PPAR- γ mediated diseases or conditions, such as osteopenia, osteoporosis, cancer, diabetes and atherosclerosis, were prepd. Thus, hydrolysis of Et 3-(cyclopropylidenemethyl)-1-[3-(trifluoromethyl)benzyl]-1H-indole-2-carboxylate (prepn. given) with NaOH in H₂O/THF afforded 57% I [R1 = 3-F₃CC₆H₄CH₂; X = O; R2 = H; R3 = cyclopropylidenemethyl; R4-R7 = H] which showed IC₅₀ of 100 pM and 9.99 nM against PPAR- γ binding.

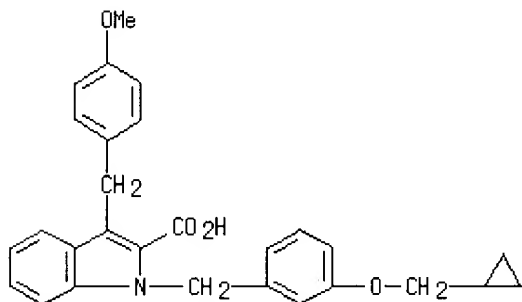
IT 412004-67-2P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of substituted indoles as PPAR- γ binding agents)

RN 412004-67-2 HCAPLUS

CN 1H-Indole-2-carboxylic acid, 1-[[3-(cyclopropylmethoxy)phenyl]methyl]-3-[(4-methoxyphenyl)methyl]- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 4 OF 5 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text	Citing References
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ACCESSION NUMBER: 2001:661388 HCAPLUS

DOCUMENT NUMBER: 135:226878

TITLE: Synthesis of N-benzyl-indolyl(benzyloxy) amido derivatives as PDE-IV inhibitors

INVENTOR(S): Labelle, Marc; Sturino, Claudio; Lachance, Nicolas; MacDonald, Dwight

PATENT ASSIGNEE(S): Merck Frosst Canada & Co., Can.

SOURCE: PCT Int. Appl., 75 pp.

CODEN: PIXXD2

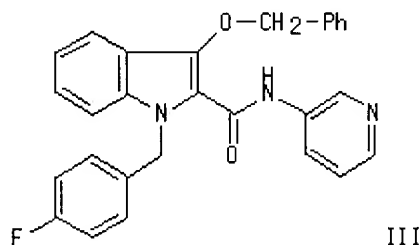
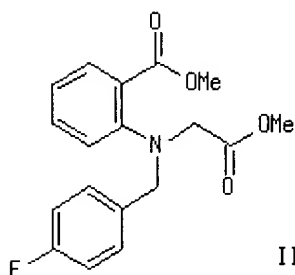
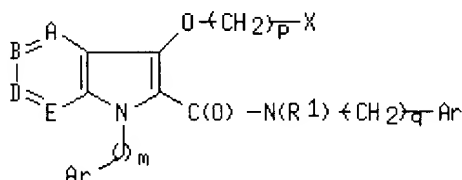
DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001064639	A2	20010907	WO 2001-CA270	20010302
WO 2001064639	A3	20020228		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
US 2002068756	A1	20020606	US 2001-797083	20010301
US 6436965	B2	20020820		
EP 1263728	A2	20021211	EP 2001-913422	20010302
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JP 2003525273	T2	20030826	JP 2001-563482	20010302
PRIORITY APPLN. INFO.:			US 2000-186571P	P 20000302
			WO 2001-CA270	W 20010302
OTHER SOURCE(S):		MARPAT 135:226878		
GI				



AB Title compds. I [A, B, D, E = N or CR₂ and the others = CR₂; q = 0 - 1; p, m = 0 - 2; R₁ = H, (hydroxy)alkyl; R₂ = H, halo, (halo)alkyl, hydroxyalkyl, CN, arom. or nonarom. ring system contg. 1 - 4 heteroatoms selected from O, S, N, alkoxy, oxyamide, etc.; X = cycloalkyl or Ar; Ar = (un)substituted (Ph, thienyl, thiazolyl, pyridyl, oxazolyl, tetrazolyl, pyrimidinyl, pyrazinyl and pyridazinyl)] were prepd. Over 150 compds. were disclosed. For instance, Me 2-aminobenzoate was alkylated with 4-fluorobenzyl bromide (K₂CO₃, MEK, reflux, 8 h.). The resulting ester was sapond. (NaOH, MeOHaq reflux, 2 h.), N-alkylated with Me bromoacetate (K₂CO₃, MeOHaq, reflux, 18 h.) and treated with CH₂N₂ to afford II. Diester II was cyclized (NaOMe, MeOH, reflux, 30 min.), O-alkylated with benzyl bromide (K₂CO₃, MEK, reflux, 2 h.), sapond. (NaOH, EtOHaq, 90°C, 40 min.) and finally coupled to 3-aminopyridine (SOCl₂, i-Pr₂NET, room temp., 3 h.) to yield III. I are PDE-IV inhibitors (no

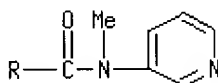
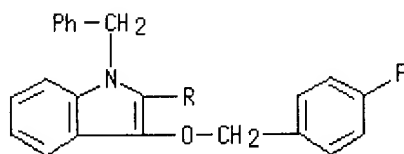
data) useful for treating, e.g., inflammation, muscle spasm, chronic bronchitis, etc.

IT **359001-30-2P**

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); **THU (Therapeutic use)**; BIOL (Biological study); PREP (Preparation); USES (Uses)
(drug; synthesis of N-benzyl-indolyl(benzyloxy)amido derivs. as PDE-IV inhibitors)

RN **359001-30-2** HCAPLUS

CN 1H-Indole-2-carboxamide, 3-[(4-fluorophenyl)methoxy]-N-methyl-1-(phenylmethyl)-N-3-pyridinyl- (9CI) (CA INDEX NAME)



L7 ANSWER 5 OF 5 HCAPLUS COPYRIGHT 2004 ACS on STN

Full
Text

Citing
References

ACCESSION NUMBER: 1999:566026 HCAPLUS
DOCUMENT NUMBER: 131:199619
TITLE: Preparation of indole derivatives as phospholipase enzyme inhibitors
INVENTOR(S): Seehra, Jasbir S.; Mckew, John C.; Lovering, Frank; Bemis, Jean E.; Xiang, Yibin; Chen, Lihren; Knopf, John L.
PATENT ASSIGNEE(S): Genetics Institute, Inc., USA
SOURCE: PCT Int. Appl., 182 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9943654	A2	19990902	WO 1999-US3898	19990224
WO 9943654	A3	19991028		
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
CA 2322162	AA	19990902	CA 1999-2322162	19990224
AU 9927825	A1	19990915	AU 1999-27825	19990224
AU 765427	B2	20030918		
BR 9908275	A	20001024	BR 1999-8275	19990224
TR 200002447	T2	20001121	TR 2000-200002447	19990224

EP 1062205	A2	20001227	EP 1999-908378	19990224
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE, FI				
JP 2002504541	T2	20020212	JP 2000-533412	19990224
EE 200000488	A	20020215	EE 2000-488	19990224
NO 2000004219	A	20001023	NO 2000-4219	20000823
HR 2000000551	A1	20010430	HR 2000-551	20000824
BG 104779	A	20011031	BG 2000-104779	20000919

PRIORITY APPLN. INFO.:

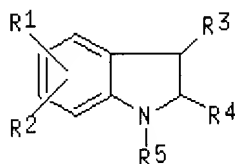
US 1998-30592 A 19980225

WO 1999-US3898 W 19990224

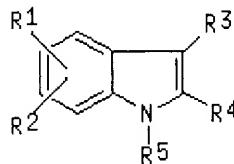
OTHER SOURCE(S):

MARPAT 131:199619

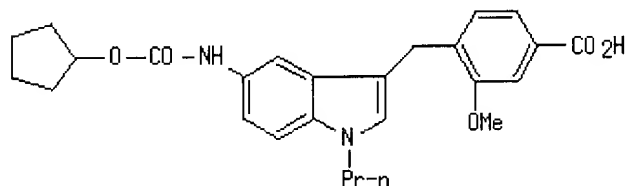
GI



I



II



III

AB Indole derivs. (I) and (II) [where R1 = H, halogen, CF₃, C1-10 alkyl, S-C1-10 alkyl, C1-10 alkoxy, CN, NO₂, NH₂, Ph, OPh, SPh, CH₂Ph, OCH₂Ph, SCH₂Ph, or (un)substituted amido, carbamido, sulfonyl, etc.; R2 = H, halogen, CF₃, OH, C1-10 alkyl, C1-10 alkoxy, CHO, CN, NO₂, (un)substituted amino, SO₂-C1-6 alkyl; R3 = (un)substituted carboxylic acid, OPO₃H₂, SO₃H, etc.; R4 = H, CF₃, C1-6 alkyl, C1-6 alkoxy, (C1-6 alkyl)cycloalkyl, CHO, halogen, etc.; R5 = C1-6 alkyl, C1-6 alkoxy, (C1-6 alkyl)cycloalkyl, etc.] and pharmaceutically acceptable salts thereof, were prep'd. by several methods. Thus, 5-nitroindole was C3-alkylated with Me 4-(bromomethyl)-3-methoxybenzoate in dioxane, N-alkylated with 1-iodopropane in a soln. of THF and NaH, and converted to the amine by hydrogenation over Pt/C. The amine was converted to the carbamate by addn. of cyclopentyl chloroformate in CH₂Cl₂ and 4-methylmorpholine and the resultant ester hydrolyzed to yield 4-[(5-[(cyclopentyloxy)carbonylamino]-1-propyl-1H-indol-3-yl)methyl]-3-methoxybenzoic acid (III). The title compds. are useful as phospholipase enzyme inhibitors, esp. cytosolic phospholipase A₂ (cPLA₂), for treatment of inflammatory conditions, particularly where inhibition of prodn. of prostaglandins, leukotrienes, and PAF are all desired. Over one hundred compds. of the invention were tested for cPLA₂ inhibiting activity in the Coumarine assay and rat carrageenan-induced footpad edema test. Compds. exhibited 7% to 98% inhibition at concns. of 0.125 μM to 400 μM in the Coumarine assay and -7.16% to 34.52% inhibition at concns. of 2 μM to 20 μM in the footpad edema test.

IT 241497-82-5P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); **THU (Therapeutic use)**;

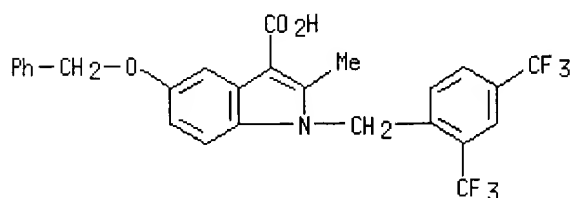
THU (Therapeutic use); BIOL (Biological study); PREP

(Preparation); RACT (Reactant or reagent); USES (Uses)

(prepn. of indole derivs. as phospholipase enzyme inhibitors for treatment of inflammatory conditions)

RN 241497-82-5 HCAPLUS

CN 1H-Indole-3-carboxylic acid, 1-[[2,4-bis(trifluoromethyl)phenyl]methyl]-2-methyl-5-(phenylmethoxy)- (9CI) (CA INDEX NAME)



=> d his

(FILE 'HOME' ENTERED AT 19:21:10 ON 22 JUN 2004)

FILE 'REGISTRY' ENTERED AT 19:21:16 ON 22 JUN 2004

L1 STRUCTURE UPLOADED

L2 4 S L1

L3 579 S L1 FULL

FILE 'HCAPLUS' ENTERED AT 19:22:04 ON 22 JUN 2004

L4 39 S L3/THU

L5 6 S L4 AND ARTHRITIS?

L6 1 S L5 AND FAULL, A?/AU

L7 5 S L5 NOT L6

=> s l4 not l5

L8 33 L4 NOT L5

=> s l8 and glomerular?

25328 GLOMERULAR?

L9 0 L8 AND GLOMERULAR?

=> s l8 and lung () fibrosis?

155142 LUNG

39674 LUNGS

168664 LUNG

(LUNG OR LUNGS)

25885 FIBROSIS?

1388 LUNG (W) FIBROSIS?

L10 0 L8 AND LUNG (W) FIBROSIS?

=> s l8 and restenosis?

5619 RESTENOSIS?

L11 2 L8 AND RESTENOSIS?

=> s l11 and faull, a?/au

34 FAULL, A?/AU

L12 0 L11 AND FAULL, A?/AU

=> s l11 and kettle, j?/au

39 KETTLE, J?/AU

L13 0 L11 AND KETTLE, J?/AU

=> d l11, ibib abs fhitr, 1-2

L11 ANSWER 1 OF 2 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text	Citing References
--------------	----------------------

ACCESSION NUMBER: 2001:319722 HCAPLUS
 DOCUMENT NUMBER: 134:320871
 TITLE: Pharmaceuticals for treating obesity containing antagonists and partial agonists of PPAR- γ
 INVENTOR(S): Berger, Joel P.; Doeber, Thomas W.; Leibowitz, Mark; Moller, David E.; Mosley, Ralph T.; Tolman, Richard L.; Ventre, John; Zhang, Bei B.; Zhou, Gaochao
 PATENT ASSIGNEE(S): Merck & Co., Inc., USA
 SOURCE: PCT Int. Appl., 49 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001030343	A1	20010503	WO 2000-US28924	20001019
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
EP 1284728	A1	20030226	EP 2000-973670	20001019
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL				
JP 2003525217	T2	20030826	JP 2001-532763	20001019
US 2003032581	A1	20030213	US 2002-241106	20020911
PRIORITY APPLN. INFO.: US 1999-161225P P 19991022 US 2000-691955 A3 20001019 WO 2000-US28924 W 20001019				

OTHER SOURCE(S): MARPAT 134:320871

AB Compds. which are antagonists of strong PPAR- γ agonists, such as rosiglitazone, and are also partial agonists of the PPAR- γ receptor, are active agents for correcting or reducing obesity. For example, 1-(p-chlorobenzyl)-5-chloro-3-thiophenylindole-2-carboxylic acid, is characterized as being a potent and selective ligand for PPAR- γ which has partial agonist (<30 maximal effects relative to rosiglitazone) and antagonist activity in cell-free and cell-based assays for the PPAR- γ receptor. The compd. is a potent agent for reducing obesity and insulin resistance in fat-fed C57BL/6J mice. This compd. and other PPAR- γ antagonists/partial agonists and pharmaceutically acceptable salts are effective in the treatment of obesity and related disorders, such as diabetes, insulin resistance, hyperlipidemia, atherosclerosis, inflammation and cancer.

IT 118414-59-8

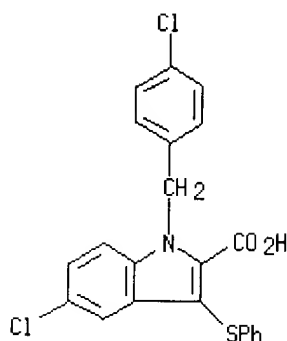
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(compns. contg. PPAR- γ receptor antagonists/partial agonists for treatment of obesity and related disorders)

RN 118414-59-8 HCAPLUS

CN 1H-Indole-2-carboxylic acid, 5-chloro-1-[(4-chlorophenyl)methyl]-3-

(phenylthio)- (9CI) (CA INDEX NAME)



REFERENCE COUNT:

5

THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 2 OF 2 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text	Citing References
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ACCESSION NUMBER: 1999:460399 HCAPLUS

DOCUMENT NUMBER: 131:87814

TITLE: Indole derivatives as inhibitors of factor Xa, and
their preparation and use as anticoagulantsINVENTOR(S): Defossa, Elisabeth; Heinelt, Uwe; Klingler, Otmar;
Zoller, Gerhard; Al-Obeidi, Fahad; Walser, Armin;
Wildgoose, Peter; Matter, Hans

PATENT ASSIGNEE(S): Hoechst Marion Roussel Deutschland GmbH, Germany

SOURCE: PCT Int. Appl., 199 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

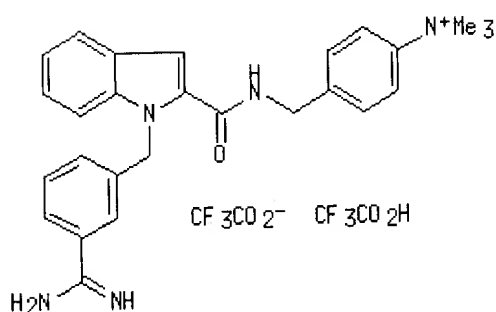
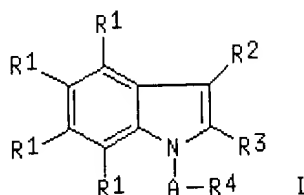
LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9933800	A1	19990708	WO 1998-EP8030	19981210
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
CA 2316172	AA	19990708	CA 1998-2316172	19981210
AU 9920528	A1	19990719	AU 1999-20528	19981210
AU 743881	B2	20020207		
BR 9814340	A	20001003	BR 1998-14340	19981210
EP 1042287	A1	20001011	EP 1998-965244	19981210
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE, SI, FI				
TR 200001954	T2	20001221	TR 2000-200001954	19981210
JP 2001527066	T2	20011225	JP 2000-526484	19981210
NZ 505370	A	20020628	NZ 1998-505370	19981210
RU 2225397	C2	20040310	RU 2000-119774	19981210
ZA 9811759	A	19990728	ZA 1998-11759	19981222

NO 2000003057 A 20000818 NO 2000-3057 20000614
 US 6337344 B1 20020108 US 2000-582344 20000814
 PRIORITY APPLN. INFO.: EP 1997-122901 A 19971224
 WO 1998-EP8030 W 19981210
 OTHER SOURCE(S): MARPAT 131:87814
 GI



AB The invention relates to the inhibition of blood clotting proteins, and more particularly, to indole derivs. or their physiol. acceptable salts which effect this, having formula I [R1 groups = H, halo, alkyl, CF3, (un)substituted Ph or phenylalkoxy, etc., with ≥ 2 of R1 being H; ≥ 1 of R2 and R3 = (CH₂)₀-2CO₂H or derivs., other = H, F, Cl, Br, or alkyl; or R₂R₃ = CH₂CH₂N(COPh)CH₂ or analogs; A = bond, alk(en/yn)ylene, CO, SO, SO₂, etc.; R₄ = (un)substituted Ph, pyridyl, or other heterocyclyl]. I are inhibitors of the blood clotting enzyme factor Xa. The invention also relates to processes for the prepn. of I, to methods of inhibiting factor Xa activity and blood clotting, to use of I in the treatment and prophylaxis of assocd. (e.g., thromboembolic) diseases, and to the use of I in the prepn. of related medicaments. The invention further relates to compns. contg. I, in particular pharmaceutical compns. contg. a compd. I and pharmaceutically acceptable carriers and/or auxiliary substances. Over 160 compds. I were prepd. For instance, 1H-indole-2-carboxylic acid Et ester underwent a 5-step sequence to give title salt II. This prepn. involved (1) N-alkylation with 3-cyanobenzyl bromide, (2) alk. hydrolysis of the ester, (3) amidation with 4-(Me₂N)C₆H₄CH₂NH₂·2HCl, (4) conversion of the nitrile to a thioamide, and (5) quaternization at dimethylamino, and ammonolysis of the thioamide to an amidine. In an assay using human factor Xa in vitro, II had a K_i value of 0.090 μ M.

IT 229950-28-1P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); **THU (Therapeutic use)**; BIOL (Biological study); PREP (Preparation); USES (Uses)
 (target compd.; prepn. of indole derivs. as inhibitors of factor Xa)

RN 229950-28-1 HCAPLUS

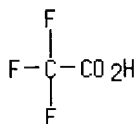
CN Pyridinium, 4-[[[1-[[3-(aminoiminomethyl)phenyl]methyl]-3-(methoxycarbonyl)-1H-indol-2-yl]carbonyl]amino]methyl]-1-methyl-, salt with trifluoroacetic acid (1:1), mono(trifluoroacetate) (9CI) (CA INDEX

NAME)

CM 1

CRN 76-05-1

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CM 2

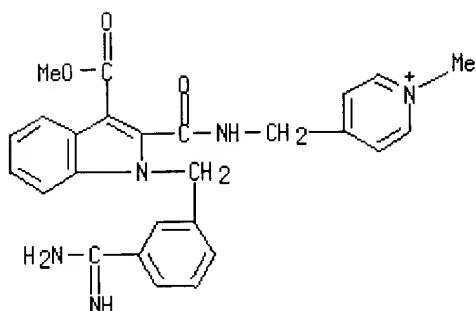
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CMF C26 H26 N5 O3 . C2 F3 O2

CM 3

CRN 229950-26-9

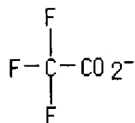
CMF C26 H26 N5 O3



CM 4

CRN 14477-72-6

CMF C2 F3 O2



REFERENCE COUNT:

2

THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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(FILE 'HOME' ENTERED AT 19:21:10 ON 22 JUN 2004)

FILE 'REGISTRY' ENTERED AT 19:21:16 ON 22 JUN 2004

L1 STRUCTURE UPLOADED

L2 4 S L1

L3 579 S L1 FULL

FILE 'HCAPLUS' ENTERED AT 19:22:04 ON 22 JUN 2004

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L4      39 S L3/THU
L5      6 S L4 AND ARTHRITIS?
L6      1 S L5 AND FAULL, A?/AU
L7      5 S L5 NOT L6
L8      33 S L4 NOT L5
L9      0 S L8 AND GLOMERULAR?
L10     0 S L8 AND LUNG () FIBROSIS?
L11     2 S L8 AND RESTENOSIS?
L12     0 S L11 AND FAULL, A?/AU
L13     0 S L11 AND KETTLE, J?/AU
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=> s l8 and alveolitis?

677 ALVEOLITIS?

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L14     0 L8 AND ALVEOLITIS?
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25401 ASTHMA?

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L15     3 L8 AND ASTHMA?
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34 FAULL, A?/AU

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L16     0 L15 AND FAULL, A?/AU
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=> s l1 and kettle, j?/au

REGISTRY INITIATED

Substance data SEARCH and crossover from CAS REGISTRY in progress...
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11.3% PROCESSED 1000 ITERATIONS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

4 ANSWERS

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 171619 TO 182901
PROJECTED ANSWERS: 352 TO 1066

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L17     4 SEA SSS SAM L1
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L18     4 L17
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L19     39 KETTLE, J?/AU
        1 L18 AND KETTLE, J?/AU
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=> file hcaplus
COST IN U.S. DOLLARS

FULL ESTIMATED COST

SINCE FILE	TOTAL
ENTRY	SESSION
2.36	208.26

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-5.54

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FILE COVERS 1907 - 22 Jun 2004 VOL 140 ISS 26
 FILE LAST UPDATED: 21 Jun 2004 (20040621/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> d his

(FILE 'HOME' ENTERED AT 19:21:10 ON 22 JUN 2004)

FILE 'REGISTRY' ENTERED AT 19:21:16 ON 22 JUN 2004

L1 STRUCTURE UPLOADED
 L2 4 S L1
 L3 579 S L1 FULL

FILE 'HCAPLUS' ENTERED AT 19:22:04 ON 22 JUN 2004

L4 39 S L3/THU
 L5 6 S L4 AND ARTHRITIS?
 L6 1 S L5 AND FAULL, A?/AU
 L7 5 S L5 NOT L6
 L8 33 S L4 NOT L5
 L9 0 S L8 AND GLOMERULAR?
 L10 0 S L8 AND LUNG () FIBROSIS?
 L11 2 S L8 AND RESTENOSIS?
 L12 0 S L11 AND FAULL, A?/AU
 L13 0 S L11 AND KETTLE, J?/AU
 L14 0 S L8 AND ALVEOLITIS?
 L15 3 S L8 AND ASTHMA?
 L16 0 S L15 AND FAULL, A?/AU
 S L1 AND KETTLE, J?/AU

FILE 'REGISTRY' ENTERED AT 19:24:50 ON 22 JUN 2004

L17 4 S L1

FILE 'HCAPLUS' ENTERED AT 19:24:51 ON 22 JUN 2004

L18 4 S L17
 L19 1 S L18 AND KETTLE, J?/AU

FILE 'HCAPLUS' ENTERED AT 19:25:00 ON 22 JUN 2004

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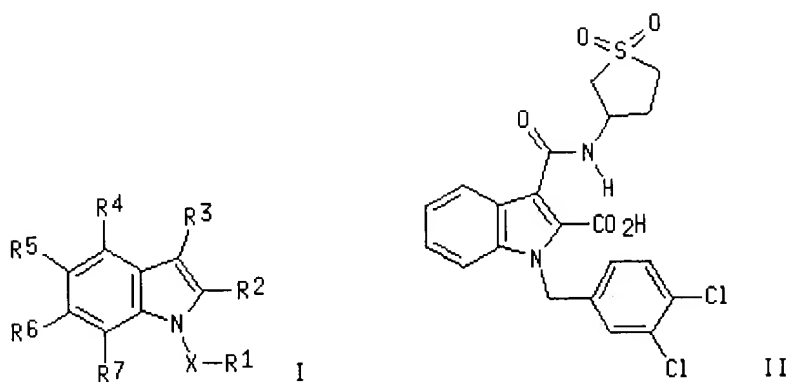
L19 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text	Citing References
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ACCESSION NUMBER: 2000:553556 HCAPLUS
 DOCUMENT NUMBER: 133:150463
 TITLE: Preparation of 3-substituted indole-2-carboxylic acids
 for the inhibition of monocyte chemoattractant
 protein-1 and/or RANTES induced chemotaxis
 INVENTOR(S): Faull, Alan Wellington; **Kettle, Jason**
 PATENT ASSIGNEE(S): Astrazeneca UK Limited, UK
 SOURCE: PCT Int. Appl., 72 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000046199	A2	20000810	WO 2000-GB284	20000131
WO 2000046199	A3	20001130		
W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG CA 2355734 AA 20000810 CA 2000-2355734 20000131 BR 2000008015 A 20011106 BR 2000-8015 20000131 EP 1173421 A2 20020123 EP 2000-901747 20000131 R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO JP 2002536362 T2 20021029 JP 2000-597270 20000131 ZA 2001005017 A 20020919 ZA 2001-5017 20010619 NO 2001003768 A 20011001 NO 2001-3768 20010801 PRIORITY APPLN. INFO.: GB 1999-2455 A 19990205 WO 2000-GB284 W 20000131				

OTHER SOURCE(S): MARPAT 133:150463
 GI



AB The title compds. [I; X = CH₂, SO₂; R₁ = (un)substituted aryl, heteroaryl; R₂ = CO₂H, CN, COCH₂OH, etc.; R₃ = OR₁₅ (wherein R₁₅ = substituted alkyl or cycloalkyl, (un)substituted heteroaryl), S(O)_qR₁₅ (q = 0-2), (CH₂)_sCO₂H (s = 0-4), etc.; R₄-R₇ = H, (un)substituted hydrocarbyl, heterocyclyl, etc.] and their pharmaceutically acceptable salts, amides or esters, useful in the prepn. of a medicament for the inhibition of monocyte chemoattractant protein-1 and/or RANTES induced chemotaxis, were prepd. and formulated. Thus, hydrolysis of the corresponding ester afforded 93% II which showed IC₅₀ of 6.86 μM against hMCP-1 receptor binding.

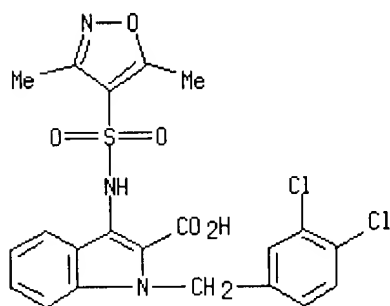
IT **287725-15-9P**

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of 3-substituted indole-2-carboxylic acids for the inhibition of monocyte chemoattractant protein-1 and/or RANTES induced chemotaxis)

RN **287725-15-9** HCAPLUS

CN 1H-Indole-2-carboxylic acid, 1-[(3,4-dichlorophenyl)methyl]-3-[[3,5-dimethyl-4-isoxazolyl)sulfonyl]amino]- (9CI) (CA INDEX NAME)



=> d his

(FILE 'HOME' ENTERED AT 19:21:10 ON 22 JUN 2004)

FILE 'REGISTRY' ENTERED AT 19:21:16 ON 22 JUN 2004

L1 STRUCTURE UPLOADED

L2 4 S L1

L3 579 S L1 FULL

FILE 'HCAPLUS' ENTERED AT 19:22:04 ON 22 JUN 2004

L4 39 S L3/THU

L5 6 S L4 AND ARTHRITIS?

L6 1 S L5 AND FAULL, A?/AU

L7 5 S L5 NOT L6
 L8 33 S L4 NOT L5
 L9 0 S L8 AND GLOMERULAR?
 L10 0 S L8 AND LUNG () FIBROSIS?
 L11 2 S L8 AND RESTENOSIS?
 L12 0 S L11 AND FAULL, A?/AU
 L13 0 S L11 AND KETTLE, J?/AU
 L14 0 S L8 AND ALVEOLITIS?
 L15 3 S L8 AND ASTHMA?
 L16 0 S L15 AND FAULL, A?/AU
 S L1 AND KETTLE, J?/AU

FILE 'REGISTRY' ENTERED AT 19:24:50 ON 22 JUN 2004

L17 4 S L1

FILE 'HCAPLUS' ENTERED AT 19:24:51 ON 22 JUN 2004

L18 4 S L17

L19 1 S L18 AND KETTLE, J?/AU

FILE 'HCAPLUS' ENTERED AT 19:25:00 ON 22 JUN 2004

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L20 3 L15 NOT L19

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L20 ANSWER 1 OF 3 HCAPLUS COPYRIGHT 2004 ACS on STN

Full
Text

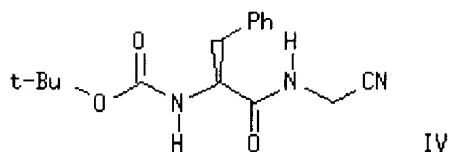
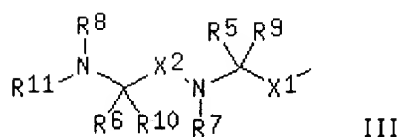
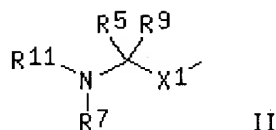
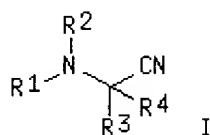
Citing
References

ACCESSION NUMBER: 2000:666700 HCAPLUS
 DOCUMENT NUMBER: 133:252170
 TITLE: Preparation of novel N-cyanomethyl amides as protease inhibitors
 INVENTOR(S): Bryant, Clifford M.; Bunin, Barry A.; Kraynack, Erica A.; Patterson, John W.
 PATENT ASSIGNEE(S): Axys Pharmaceuticals, Inc., USA
 SOURCE: PCT Int. Appl., 137 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 2
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000055125	A2	20000921	WO 2000-US6747	20000315
WO 2000055125	A3	20010426		
W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG BR 2000009042 A 20011226 BR 2000-9042 20000315 EP 1178958 A2 20020213 EP 2000-916343 20000315 EP 1178958 B1 20040218 R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,				

IE, SI, LT, LV, FI, RO			
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TR 200103390	T2	20020521	TR 2001-20010339020000315
US 6455502	B1	20020924	US 2000-526090 20000315
TR 200201874	T2	20021021	TR 2002-20020187420000315
US 6476026 - NO	B1	20021105	US 2000-526485 20000315
JP 2002539191	T2	20021119	JP 2000-605556 20000315
EE 200100485	A	20030217	EE 2001-485 20000315
NZ 514234	A	20040227	NZ 2000-514234 20000315
AT 259782	E	20040315	AT 2000-916343 20000315
ZA 2001007494	A	20020911	ZA 2001-7494 20010911
ZA 2001007495	A	20020911	ZA 2001-7495 20010911
NO 2001004485	A	20011105	NO 2001-4485 20010914
BG 106003	A	20020628	BG 2001-106003 20011010
HR 2001000738	A1	20021231	HR 2001-738 20011012
US 2002086996 - NO	A1	20020704	US 2001-17851 20011214
US 6593327 - NO	B2	20030715	
US 2003096796 - NO	A1	20030522	US 2002-205600 20020724
US 2003119788 - NO	A1	20030626	US 2002-241001 20020909
PRIORITY APPLN. INFO.:			
			US 1999-124420P P 19990315
			US 2000-526090 A1 20000315
			US 2000-526485 A3 20000315
			WO 2000-US6747 W 20000315

OTHER SOURCE(S): MARPAT 133:252170
GI



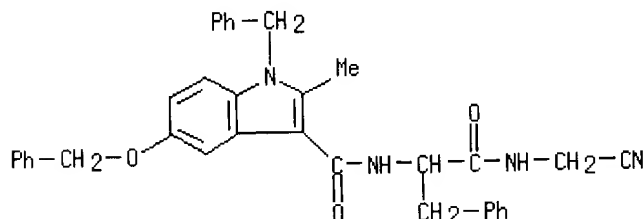
AB The title compds. [I; R1 = II, III (wherein X1, X2 = CO, CH2SO2; R5, R6 = H, alkyl; R7, R8 = H, alkyl, etc.; R9, R10 = alkyl optionally substituted with CN, halo, NO2, etc.; R11 = X5X6R18; X5 = CO, COCO, SO2; X6 = a bond, O, NH, N(alkyl); R18 = alkyl optionally substituted with CN, halo, NO2, etc.); R2 = H, alkyl, etc.; R3 = H, alkyl, etc.; R4 = H, alkyl optionally substituted with CN, halo, NO2, etc.; R4 and R2 taken together form trimethylene, tetramethylene, phenylene-1,2-dimethylene, optionally substituted with hydroxy, oxo or methylene; R4 and R3 together with the carbon atom to which both are attached form cycloalkylene, heterocycloalkylene], useful for treating diseases assocd. with cysteine protease activity, particularly diseases assocd. with activity of cathepsins B, K, L or S such as inflammation and **asthma**, were prepd. and formulated. Thus, reacting 2(S)-tert-butoxycarbonylamino-3-phenylpropionic acid with aminoacetonitrile.HCl in the presence of Et3N DMF and MeCN afforded the amide (1S)-IV. Biol. data for compds. I were given.

IT **294640-68-9P**

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); **THU (Therapeutic use)**; BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of novel N-cyanomethyl amides as protease inhibitors)

RN 294640-68-9 HCAPLUS

CN 1H-Indole-3-carboxamide, N-[2-[(cyanomethyl)amino]-2-oxo-1-(phenylmethyl)ethyl]-2-methyl-5-(phenylmethoxy)-1-(phenylmethyl)- (9CI)
(CA INDEX NAME)



L20 ANSWER 2 OF 3 HCAPLUS COPYRIGHT 2004 ACS on STN

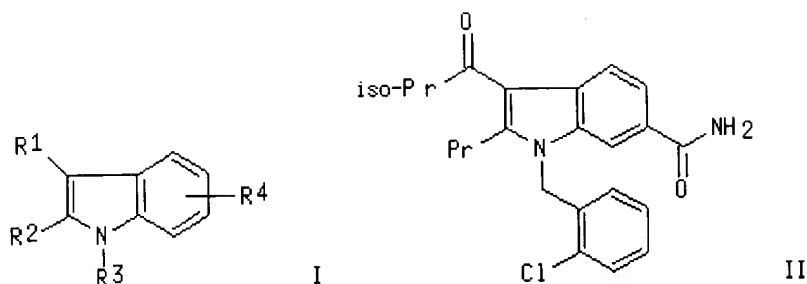
Full Text Citing References

ACCESSION NUMBER: 1996:746234 HCAPLUS
DOCUMENT NUMBER: 126:18786
TITLE: Indole derivatives as cGMP-PDE inhibitors
INVENTOR(S): Oku, Teruo; Sawada, Kozo; Kuroda, Akio; Ohne, Kazuhiko; Nomoto, Atsushi; Hosogai, Naomi; Nakajima, Yoshimitsu; Nagashima, Akira; Sogabe, Keizo; Amura, Kouichi
PATENT ASSIGNEE(S): Fujisawa Pharmaceutical Co, Ltd., Japan
SOURCE: PCT Int. Appl., 211 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

none of the examples read

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9632379	A1	19961017	WO 1996-JP892	19960402
CA 2217707	AA	19961017	CA 1996-2217707	19960402
AU 9651234	A1	19961030	AU 1996-51234	19960402
AU 713460	B2	19991202		
EP 820441	A1	19980128	EP 1996-907750	19960402
EP 820441	B1	20020626		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE, FI				
CN 1187812	A	19980715	CN 1996-194691	19960402
JP 11503445	T2	19990326	JP 1996-530864	19960402
AT 219765	E	20020715	AT 1996-907750	19960402
ES 2175079	T3	20021116	ES 1996-907750	19960402
ZA 9602859	A	19961011	ZA 1996-2859	19960410
TW 420663	B	20010201	TW 1996-85104519	19960416
US 6069156	A	20000530	US 1997-930597	19971210
PRIORITY APPLN. INFO.:				
			GB 1995-7432	A 19950410
			GB 1995-12560	A 19950621
			GB 1995-16136	A 19950807
			AU 1996-8294	A 19960227
			WO 1996-JP892	W 19960402

OTHER SOURCE(S): MARPAT 126:18786
GI



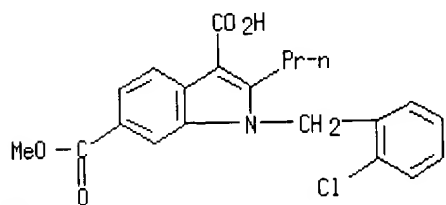
AB The invention relates to new indole derivs. I and their pharmaceutically acceptable salts [wherein R1 = H, halo, NO₂, CO₂H, protected CO₂H, acyl, (un)substituted alk(en)yl, etc.; R2 = H, halo, alkenyl, acyl, (un)substituted alkyl, etc.; R3 = (un)substituted alk(en)yl where the substituent is oxo, (un)substituted aryl, or heterocyclyl; R4 = CO₂H, protected CO₂H, acyl, cyano, amino, halo, etc.; R1 and R2 may form 4- to 7-membered carboxylic ring (un)substituted with oxo]. I are cyclic nucleotide-PDE inhibitors (specifically cGMP-PDE), and are useful for treating and preventing a variety of conditions, including angina, hypertension, renal failure, atherosclerosis, stroke, **asthma**, impotence, diabetic complications, and glaucoma. Almost 300 compds. I and numerous intermediates were prepd. For example, Me 3-isobutyryl-2-propylindole-6-carboxylate (prepn. given) was N-benzylated by 2-chlorobenzyl bromide using NaH in DMF. The product underwent sapon. with NaOH in aq. EtOH, followed by amidation of the resultant acid using EDC, HOBt, and aq. NH₃, to give title amide II. II inhibited human platelet cGMP-PDE in vitro with IC₅₀ <100 nM. I were also active in a variety of other bioassays, including relaxation of isolated rat aorta, inhibition of vascular smooth muscle cell proliferation, inhibition of vasopressin-induced vasospasm, the cyclosporin and FK506 nephritis models, the diabetic glomerulosclerosis model, and several animal impotence models.

IT **184149-02-8P**

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); **THU (Therapeutic use)**; **THU (Therapeutic use)**; BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses) (prepn. of indole derivs. as cGMP-PDE inhibitors)

RN **184149-02-8** HCAPLUS

CN 1H-Indole-3,6-dicarboxylic acid, 1-[(2-chlorophenyl)methyl]-2-propyl-, 6-methyl ester (9CI) (CA INDEX NAME)



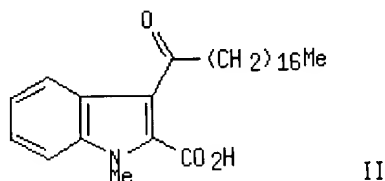
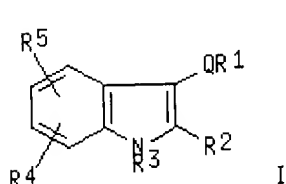
L20 ANSWER 3 OF 3 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text Citing References

ACCESSION NUMBER: 1995:638471 HCAPLUS
DOCUMENT NUMBER: 123:32958

TITLE: Indole-2-alkanoic acids and their derivatives as inhibitors of phospholipase A2.
 INVENTOR(S): Lehr, Matthias
 PATENT ASSIGNEE(S): Germany
 SOURCE: Ger. Offen., 30 pp.
 CODEN: GWXXBX
 DOCUMENT TYPE: Patent
 LANGUAGE: German
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 4338770	A1	19950518	DE 1993-4338770	19931112
WO 9513266	A1	19950518	WO 1994-DE1121	19940920
W: AM, AU, BB, BG, BR, BY, CA, CN, CZ, EE, FI, GE, HU, JP, KG, KP, KR, KZ, LK, LR, LT, LV, MD, MG, MN, NO, NZ, PL, RO, RU, SI, SK, TJ, TT, UA, US, UZ, VN				
RW: KE, MW, SD, SZ, AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
AU 9476907	A1	19950529	AU 1994-76907	19940920
PRIORITY APPLN. INFO.:			DE 1993-4338770	19931112
			WO 1994-DE1121	19940920
OTHER SOURCE(S):			MARPAT 123:32958	
GI				

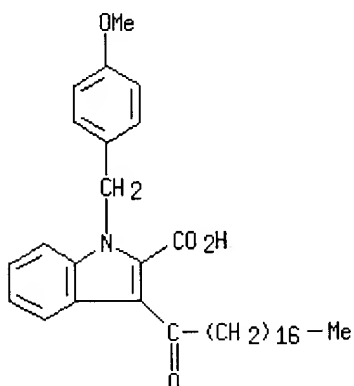


AB Title compds. I [R1 = X, (un)substituted aryl, -X-aryl; X = C1-19 alk(en/yn)yl optionally interrupted by O; R2 = CO2H, -Y-CO2H, Tz, -Y-Tz; Y = C1-8 alk(en)yl optionally interrupted by O; Tz = 1H- or 2H-tetrazol-5-yl; R3 = H, Z (Z = C1-20 alk(en/yn)yl optionally interrupted by O), (un)substituted aryl or -Z-aryl, or Z (un)substituted by OH, acyloxy, SH, acylthio, NH2, or acylamino; Q = CO, CH2, (acylamino)methylene; R4, R5 = H, as given for Z, halo, CF3, OH, cyano, many others] and their pharmaceutical salts and esters are claimed. The compds. are inhibitors of phospholipase A2 (PLA2), and are claimed useful for treatment or prevention of inflammation, allergy, **asthma**, psoriasis, and endotoxin shock. For example, acylation of indole-2-carboxylic acid Et ester with octadecanoic acid in CH2Cl2 in the presence of polyphosphoric acid and (CF3CO)2O gave 42% 3-octadecanoyl deriv., which was N-alkylated by p-MeC6H4SO3Me under phase-transfer conditions (75%) and hydrolyzed by aq. KOH in refluxing EtOH (80%) to give title compd. II. In a test for inhibition of PLA2 using bovine platelets in vitro, II at 10 μ M gave 61% inhibition, vs. only 42% for the known inhibitor (S)-N-hexadecyl-2-pyrrolidinecarboxamide.

IT 164160-85-4P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); **THU (Therapeutic use)**; **THU (Therapeutic use)**; BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses) (prepn. of indolealkanoic acids as phospholipase A2 inhibitors)

RN 164160-85-4 HCAPLUS
 CN 1H-Indole-2-carboxylic acid, 1-[(4-methoxyphenyl)methyl]-3-(1-oxooctadecyl)- (9CI) (CA INDEX NAME)



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(FILE 'HOME' ENTERED AT 19:21:10 ON 22 JUN 2004)

FILE 'REGISTRY' ENTERED AT 19:21:16 ON 22 JUN 2004

L1 STRUCTURE UPLOADED
 L2 4 S L1
 L3 579 S L1 FULL

FILE 'HCAPLUS' ENTERED AT 19:22:04 ON 22 JUN 2004

L4 39 S L3/THU
 L5 6 S L4 AND ARTHRITIS?
 L6 1 S L5 AND FAULL, A?/AU
 L7 5 S L5 NOT L6
 L8 33 S L4 NOT L5
 L9 0 S L8 AND GLOMERULAR?
 L10 0 S L8 AND LUNG () FIBROSIS?
 L11 2 S L8 AND RESTENOSIS?
 L12 0 S L11 AND FAULL, A?/AU
 L13 0 S L11 AND KETTLE, J?/AU
 L14 0 S L8 AND ALVEOLITIS?
 L15 3 S L8 AND ASTHMA?
 L16 0 S L15 AND FAULL, A?/AU
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FILE 'REGISTRY' ENTERED AT 19:24:50 ON 22 JUN 2004

L17 4 S L1

FILE 'HCAPLUS' ENTERED AT 19:24:51 ON 22 JUN 2004

L18 4 S L17
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FILE 'HCAPLUS' ENTERED AT 19:25:00 ON 22 JUN 2004

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39766 ATHEROSCLEROSIS?

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L22 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text	Citing References
--------------	----------------------

ACCESSION NUMBER:	2001:319722 HCAPLUS
DOCUMENT NUMBER:	134:320871
TITLE:	Pharmaceuticals for treating obesity containing antagonists and partial agonists of PPAR- γ
INVENTOR(S):	Berger, Joel P.; Doebber, Thomas W.; Leibowitz, Mark; Moller, David E.; Mosley, Ralph T.; Tolman, Richard L.; Ventre, John; Zhang, Bei B.; Zhou, Gaochao
PATENT ASSIGNEE(S):	Merck & Co., Inc., USA
SOURCE:	PCT Int. Appl., 49 pp. CODEN: PIXXD2
DOCUMENT TYPE:	Patent
LANGUAGE:	English
FAMILY ACC. NUM. COUNT:	1
PATENT INFORMATION:	

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001030343	A1	20010503	WO 2000-US28924	20001019
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
EP 1284728	A1	20030226	EP 2000-973670	20001019
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL				
JP 2003525217	T2	20030826	JP 2001-532763	20001019
US 2003032581	A1	20030213	US 2002-241106	20020911
US 1999-161225P P 19991022 US 2000-691955 A3 20001019 WO 2000-US28924 W 20001019				

PRIORITY APPLN. INFO.: MARPAT 134:320871

AB Comps. which are antagonists of strong PPAR- γ agonists, such as rosiglitazone, and are also partial agonists of the PPAR- γ receptor, are active agents for correcting or reducing obesity. For example, 1-(p-chlorobenzyl)-5-chloro-3-thiophenylindole-2-carboxylic acid, is characterized as being a potent and selective ligand for PPAR- γ which has partial agonist (<30 maximal effects relative to rosiglitazone) and antagonist activity in cell-free and cell-based assays for the PPAR- γ receptor. The compd. is a potent agent for reducing obesity

and insulin resistance in fat-fed C57BL/6J mice. This compd. and other PPAR- γ antagonists/partial agonists and pharmaceutically acceptable salts are effective in the treatment of obesity and related disorders, such as diabetes, insulin resistance, hyperlipidemia, **atherosclerosis**, inflammation and cancer.

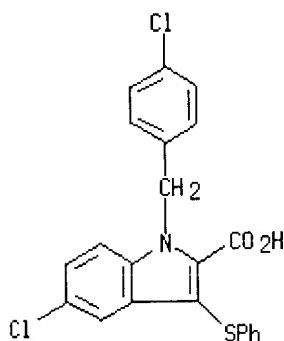
IT **118414-59-8**

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); **THU (Therapeutic use)**; BIOL (Biological study); USES (Uses)

(compns. contg. PPAR- γ receptor antagonists/partial agonists for treatment of obesity and related disorders)

RN **118414-59-8** HCAPLUS

CN 1H-Indole-2-carboxylic acid, 5-chloro-1-[(4-chlorophenyl)methyl]-3-(phenylthio)- (9CI) (CA INDEX NAME)



REFERENCE COUNT:

5

THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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(FILE 'HOME' ENTERED AT 19:21:10 ON 22 JUN 2004)

FILE 'REGISTRY' ENTERED AT 19:21:16 ON 22 JUN 2004

L1 STRUCTURE UPLOADED

L2 4 S L1

L3 579 S L1 FULL

FILE 'HCAPLUS' ENTERED AT 19:22:04 ON 22 JUN 2004

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L5 6 S L4 AND ARTHRITIS?

L6 1 S L5 AND FAULL, A?/AU

L7 5 S L5 NOT L6

L8 33 S L4 NOT L5

L9 0 S L8 AND GLOMERULAR?

L10 0 S L8 AND LUNG () FIBROSIS?

L11 2 S L8 AND RESTENOSIS?

L12 0 S L11 AND FAULL, A?/AU

L13 0 S L11 AND KETTLE, J?/AU

L14 0 S L8 AND ALVEOLITIS?

L15 3 S L8 AND ASTHMA?

L16 0 S L15 AND FAULL, A?/AU

S L1 AND KETTLE, J?/AU

FILE 'REGISTRY' ENTERED AT 19:24:50 ON 22 JUN 2004

L17 4 S L1

FILE 'HCAPLUS' ENTERED AT 19:24:51 ON 22 JUN 2004

L18 4 S L17
L19 1 S L18 AND KETTLE, J?/AU

FILE 'HCAPLUS' ENTERED AT 19:25:00 ON 22 JUN 2004

L20 3 S L15 NOT L19
L21 30 S L8 NOT L20
L22 1 S L21 AND ATHEROSCLEROSIS?
L23 0 S L22 AND FAULL, A?/AU
L24 0 S L22 AND KETTLE, J?/AU

=> s 121 not 122
L25 29 L21 NOT L22

=> s 125 and skin?
213767 SKIN?
L26 2 L25 AND SKIN?

=> s 126 and faull, a?/au
34 FAULL, A?/AU
L27 0 L26 AND FAULL, A?/AU

=> s 125 and kettle, j?/au
39 KETTLE, J?/AU
L28 3 L25 AND KETTLE, J?/AU

=> s 126 and kettle, j?/au
39 KETTLE, J?/AU
L29 0 L26 AND KETTLE, J?/AU

=> d 126, ibib abs fhitrstr, 1-2

L26 ANSWER 1 OF 2 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text	Citing References
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ACCESSION NUMBER:	2003:551494 HCAPLUS
DOCUMENT NUMBER:	139:101027
TITLE:	Preparation of mercaptoethyl indolecarboxylic acids as NAALAdase inhibitors for treating and diagnosing glutamate abnormalities, neurological and other disorders
INVENTOR(S):	Tsukamoto, Takashi; Grella, Brian; Majer, Pavel
PATENT ASSIGNEE(S):	Guilford Pharmaceuticals Inc., USA
SOURCE:	PCT Int. Appl., 173 pp. CODEN: PIXXD2
DOCUMENT TYPE:	Patent
LANGUAGE:	English
FAMILY ACC. NUM. COUNT:	1
<u>PATENT INFORMATION:</u>	

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003057670	A2	20030717	WO 2002-US37617	20021219
WO 2003057670	A3	20031106		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD,				

RU, TJ, TM

RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG,
CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL,
PT, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML,
MR, NE, SN, TD, TG

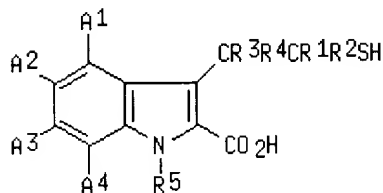
PRIORITY APPLN. INFO.:

US 2001-342764P P 20011228

OTHER SOURCE(S):

MARPAT 139:101027

GI



AB This invention relates to new indoles (shown as I; variables defined below; e.g. 3-(2-mercaptoethyl)-1H-indole-2-carboxylic acid), pharmaceutical compns. and diagnostic kits comprising such compds., and methods of using such compds. for inhibiting NAALADase enzyme activity, detecting diseases where NAALADase levels are altered, affecting neuronal activity, effecting TGF- β activity, inhibiting angiogenesis, and treating glutamate abnormalities, neuropathy, pain, compulsive disorders, prostate diseases, cancers and glaucoma. IC50 values are tabulated for inhibition of NAALADase by 12 examples of I. Many pharmacol. and therapeutic test results are reported for the following 6 compds. that are not covered by I: 2-[[[(2,3,4,5,6-pentafluorobenzyl)hydroxyphosphinyl]methyl]pentanedioic acid, 2-(3-sulfanylpropyl)pentanedioic acid, 2-(phosphonomethyl)pentanedioic acid, 2-(2-sulfanylethyl)pentanedioic acid, 3-carboxy- α -(3-mercaptopropyl)benzenepropanoic acid and 3-carboxy-5-(1,1-dimethylethyl)- α -(3-mercaptopropyl)benzenepropanoic acid. For I: A1, A2, A3 and A4 = H, C1-C9 alkyl, C2-C9 alkenyl, C2-C9 alkynyl, aryl, heteroaryl, carbocycle, heterocycle, C1-C9 alkoxy, C2-C9 alkenyloxy, phenoxy, benzyloxy, hydroxy, halo, nitro, cyano, isocyano, -COOR6, -COR6, -NR6R7, -SR6, -SOR6, -SO2R6, -SO2(OR6), -C(O)NR6R7, -C(O)NR6 (CH2)nCOOH, -NR6C(O)R7 or -(CH2)nCOOH, or any adjacent two of A1, A2, A3 and A4 form with the benzene ring a fused ring that is (un)satd., arom. or nonarom., and carbocyclic or heterocyclic, said heterocyclic ring contg. 1 or 2 O, N and/or S heteroatom(s); n is 1-3; R, R1, R2, R3, R4, R5, R6, R7 = H, carboxy, C1-C9 alkyl, C2-C9 alkenyl, C2-C9 alkynyl, aryl, heteroaryl, carbocycle or heterocycle; and said alkyl, alkenyl, alkynyl, aryl, heteroaryl, carbocycle, heterocycle, alkoxy, alkenyloxy, phenoxy, benzyloxy and fused ring (un)substituted with ≥ 1 substituent(s). Although the methods of prepn. are not claimed, 13 example preps. are included.

IT **560131-44-4P**, 1-[(3-Carboxyphenyl)methyl]-3-(2-mercaptoethyl)-1H-indole-2-carboxylic acid

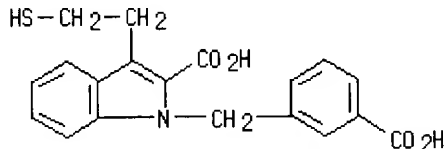
RL: DGN (Diagnostic use); PAC (Pharmacological activity); SPN (Synthetic preparation); **THU (Therapeutic use)**; BIOL (Biological study); PREP (Preparation); USES (Uses)

(drug candidate and diagnosis agent; prepn. of mercaptoethyl indolecarboxylic acids as NAALADase inhibitors for treating and diagnosing glutamate abnormalities and neurol. and other disorders)

RN **560131-44-4** HCAPLUS

CN 1H-Indole-2-carboxylic acid, 1-[(3-carboxyphenyl)methyl]-3-(2-

mercaptoethyl)- (9CI) (CA INDEX NAME)



L26 ANSWER 2 OF 2 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text	Citing References
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ACCESSION NUMBER: 1995:994335 HCAPLUS
 DOCUMENT NUMBER: 124:86811
 TITLE: Novel indole derivatives useful to treat estrogen-related neoplasms and disorders
 INVENTOR(S): Bitonti, Alan J.; McDonald, Ian A.; Salituro, Francesco G.; Whitten, Jeffrey P.; Jarvi, Esa T.; Wright, Paul S.
 PATENT ASSIGNEE(S): Merrell Dow Pharmaceuticals Inc., USA
 SOURCE: PCT Int. Appl., 173 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

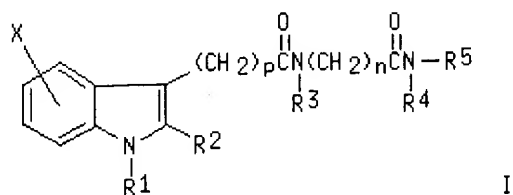
NO Examples

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9522524	A1	19950824	WO 1995-US1372	19950131
W: AM, AT, AU, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, ES, FI, GB, GE, HU, JP, KE, KG, KP, KR, KZ, LK, LT, LU, LV, MD, MG, MN, MW, NL, NO, NZ, PL, PT, RO, RU, SD, SE, SI, SK, TJ, TT, UA, US, US, UZ, VN RW: KE, MW, SD, SZ, AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
CA 2183731	AA	19950824	CA 1995-2183731	19950131
AU 9518373	A1	19950904	AU 1995-18373	19950131
AU 680740	B2	19970807		
EP 746544	A1	19961211	EP 1995-910164	19950131
EP 746544	B1	19980909		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE				
CN 1141627	A	19970129	CN 1995-191750	19950131
HU 76133	A2	19970630	HU 1996-2299	19950131
JP 09509169	T2	19970916	JP 1995-521822	19950131
JP 3536258	B2	20040607		
AT 170839	E	19980915	AT 1995-910164	19950131
ES 2122555	T3	19981216	ES 1995-910164	19950131
ZA 9501297	A	19951024	ZA 1995-1297	19950216
US 5877202	A	19990302	US 1996-594505	19960131
FI 9603272	A	19960821	FI 1996-3272	19960821
NO 9603483	A	19961022	NO 1996-3483	19960821

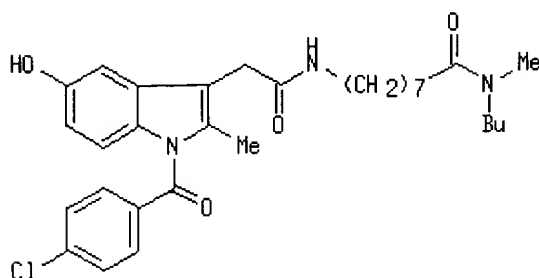
PRIORITY APPLN. INFO.:

US 1994-200057	A2	19940222
US 1994-362046	A2	19941222
WO 1995-US1372	W	19950131

OTHER SOURCE(S): MARPAT 124:86811
 GI



I



II

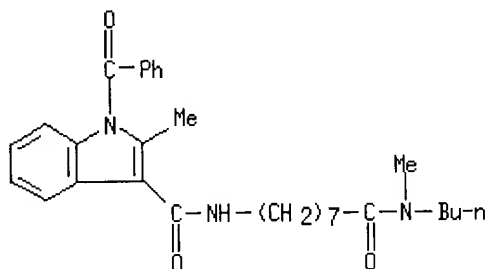
AB The invention relates to indole derivs. I [$n = 1-12$; $p = 0, 1$; $X = 1-3$ of H, halo, OH, alkyl, alkoxy, R_6CO_2 ; $R_1 = H$, alkyl, (un)substituted phenylalkyl, benzoyl, carbamoyl, etc.; $R_2 = H$, alkyl, (un)substituted Ph; $R_3, R_4 = H$, alkyl; $R_5 = H$, alkyl, Ph; or $R_4R_5 = CH_2CH_2GCH_2CH_2$; $G = \text{bond, NMe, } CH_2, O$; $R_6 = \text{alkyl, (un)substituted Ph}$; one of $R_1-R_5 \neq H$ when $n = 1$] and their pharmaceutically acceptable salts. I and salts are useful in down-regulating estrogen receptor expression. Also included are methods for the treatment or prophylaxis of neoplasms or of controlling neoplasm growth, esp. estrogen-dependent neoplasms such as those assocd. with breast, ovarian, and cervical tissue. Also provided is a method for treating autoimmune diseases. For example, reaction of 1-[5-methoxy-1-(4-chlorobenzoyl)-2-methyl-1H-indol-3-yl]acetic acid chloride with 8-aminooctanoic acid methylbutylamide [prepn. given] in PhMe in the presence of (iso-Pr) $_2$ NEt, and demethylation of the phenolic Me ether with BBr $_3$ in CH_2Cl_2 , gave the preferred compd. II [also named MDL 101,906]. The latter inhibited estradiol-dependent transcription of an estradiol-dependent luciferase reporter plasmid in MCF-7 human breast tumor cells with an IC_{50} of 5.2 μM . Over 180 synthetic examples cover prepn. of I and intermediates, and 9 biol. examples cover a variety of tests of selected I, including relative binding affinities to estrogen receptor, depletion of receptor from tumor cells, and inhibition of cells including tamoxifen-resistant LY-2 cells (IC_{50} of II = 4.7 μM).

IT 172595-48-1P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); **THU (Therapeutic use)**; BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of indoles as estrogen-dependent antineoplastics)

RN 172595-48-1 HCAPLUS

CN 1H-Indole-3-carboxamide, 1-benzoyl-N-[8-(butylmethylamino)-8-oxooctyl]-2-methyl- (9CI) (CA INDEX NAME)



=> d his

(FILE 'HOME' ENTERED AT 19:21:10 ON 22 JUN 2004)

FILE 'REGISTRY' ENTERED AT 19:21:16 ON 22 JUN 2004

L1 STRUCTURE UPLOADED

L2 4 S L1

L3 579 S L1 FULL

FILE 'HCAPLUS' ENTERED AT 19:22:04 ON 22 JUN 2004

L4 39 S L3/THU

L5 6 S L4 AND ARTHRITIS?

L6 1 S L5 AND FAULL, A?/AU

L7 5 S L5 NOT L6

L8 33 S L4 NOT L5

L9 0 S L8 AND GLOMERULAR?

L10 0 S L8 AND LUNG () FIBROSIS?

L11 2 S L8 AND RESTENOSIS?

L12 0 S L11 AND FAULL, A?/AU

L13 0 S L11 AND KETTLE, J?/AU

L14 0 S L8 AND ALVEOLITIS?

L15 3 S L8 AND ASTHMA?

L16 0 S L15 AND FAULL, A?/AU

S L1 AND KETTLE, J?/AU

FILE 'REGISTRY' ENTERED AT 19:24:50 ON 22 JUN 2004

L17 4 S L1

FILE 'HCAPLUS' ENTERED AT 19:24:51 ON 22 JUN 2004

L18 4 S L17

L19 1 S L18 AND KETTLE, J?/AU

FILE 'HCAPLUS' ENTERED AT 19:25:00 ON 22 JUN 2004

L20 3 S L15 NOT L19

L21 30 S L8 NOT L20

L22 1 S L21 AND ATHEROSCLEROSIS?

L23 0 S L22 AND FAULL, A?/AU

L24 0 S L22 AND KETTLE, J?/AU

L25 29 S L21 NOT L22

L26 2 S L25 AND SKIN?

L27 0 S L26 AND FAULL, A?/AU

L28 3 S L25 AND KETTLE, J?/AU

L29 0 S L26 AND KETTLE, J?/AU

=> s 125 not 126

L30 27 L25 NOT L26

=> s 130 and multiple () sclerosis?

325687 MULTIPLE
 3005 MULTIPLES
 328373 MULTIPLE
 (MULTIPLE OR MULTIPLES)
 18498 SCLEROSIS?
 10942 MULTIPLE (W) SCLEROSIS?
 L31 0 L30 AND MULTIPLE (W) SCLEROSIS?

=> s 130 and inflamm? () bowel?
 183147 INFLAMM?
 11651 BOWEL?
 4273 INFLAMM? (W) BOWEL?
 L32 0 L30 AND INFLAMM? (W) BOWEL?

=> s 130 and brain () trauma?
 462841 BRAIN
 21566 BRAINS
 465094 BRAIN
 (BRAIN OR BRAINS)
 17295 TRAUMA?
 826 BRAIN (W) TRAUMA?
 L33 1 L30 AND BRAIN (W) TRAUMA?

=> d 133, ibib abs fhitr, 1

L33 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text	Citing References
ACCESSION NUMBER:	1998:635621 HCAPLUS
DOCUMENT NUMBER:	129:265475
TITLE:	Indolecarboxamides, preparation thereof, pharmaceutical compositions, and methods of inhibiting calpain
INVENTOR(S):	Daines, Robert A.; Sham, Kelvin Kin-Cheong
PATENT ASSIGNEE(S):	Smithkline Beecham Corp., USA
SOURCE:	PCT Int. Appl., 17 pp. CODEN: PIXXD2
DOCUMENT TYPE:	Patent
LANGUAGE:	English
FAMILY ACC. NUM. COUNT:	1
PATENT INFORMATION:	

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9841092	A1	19980924	WO 1998-US4873	19980313
W: CA, JP, US				
RW: AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
EP 1018878	A1	20000719	EP 1998-909146	19980313
R: BE, CH, DE, ES, FR, GB, IT, LI, NL				
JP 2001515508	T2	20010918	JP 1998-540629	19980313
US 6214856	B1	20010410	US 1999-380317	19990830
PRIORITY APPLN. INFO.:			US 1997-40589P	P 19970314
			WO 1998-US4873	W 19980313

OTHER SOURCE(S): MARPAT 129:265475
 AB Pharmaceutical compns. and methods of inhibiting calpain using indolecarboxamides are disclosed. The compns. and methods of the invention are useful in the treatment of e.g. neurodegenerative disorders, strokes, and traumatic brain injury. Prepn. of e.g. (S)-N-(1-formyl-2-phenylethyl)-1-methyl-2-indolecarboxamide is described, as are capsule and other formulations.

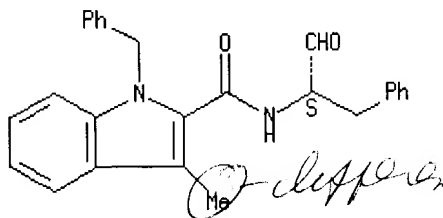
IT 213599-01-0P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); **THU (Therapeutic use)**; BIOL (Biological study); PREP (Preparation); USES (Uses)
(indolecarboxamides, prepn., pharmaceutical compns., and methods of inhibiting calpain)

RN 213599-01-0 HCAPLUS

CN 1H-Indole-2-carboxamide, N-[(1S)-1-formyl-2-phenylethyl]-3-methyl-1-(phenylmethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT:

2

THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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(FILE 'HOME' ENTERED AT 19:21:10 ON 22 JUN 2004)

FILE 'REGISTRY' ENTERED AT 19:21:16 ON 22 JUN 2004

L1 STRUCTURE UPLOADED

L2 4 S L1

L3 579 S L1 FULL

FILE 'HCAPLUS' ENTERED AT 19:22:04 ON 22 JUN 2004

L4 39 S L3/THU

L5 6 S L4 AND ARTHRITIS?

L6 1 S L5 AND FAULL, A?/AU

L7 5 S L5 NOT L6

L8 33 S L4 NOT L5

L9 0 S L8 AND GLOMERULAR?

L10 0 S L8 AND LUNG () FIBROSIS?

L11 2 S L8 AND RESTENOSIS?

L12 0 S L11 AND FAULL, A?/AU

L13 0 S L11 AND KETTLE, J?/AU

L14 0 S L8 AND ALVEOLITIS?

L15 3 S L8 AND ASTHMA?

L16 0 S L15 AND FAULL, A?/AU

S L1 AND KETTLE, J?/AU

FILE 'REGISTRY' ENTERED AT 19:24:50 ON 22 JUN 2004

L17 4 S L1

FILE 'HCAPLUS' ENTERED AT 19:24:51 ON 22 JUN 2004

L18 4 S L17

L19 1 S L18 AND KETTLE, J?/AU

FILE 'HCAPLUS' ENTERED AT 19:25:00 ON 22 JUN 2004

L20 3 S L15 NOT L19

L21 30 S L8 NOT L20

L22 1 S L21 AND ATHEROSCLEROSIS?

L23 0 S L22 AND FAULL, A?/AU

L24 0 S L22 AND KETTLE, J?/AU
 L25 29 S L21 NOT L22
 L26 2 S L25 AND SKIN?
 L27 0 S L26 AND FAULL, A?/AU
 L28 3 S L25 AND KETTLE, J?/AU
 L29 0 S L26 AND KETTLE, J?/AU
 L30 27 S L25 NOT L26
 L31 0 S L30 AND MULTIPLE () SCLEROSIS?
 L32 0 S L30 AND INFLAMM? () BOWEL?
 L33 1 S L30 AND BRAIN () TRAUMA?

=> s 130 not 133

L34 26 L30 NOT L33

=> s 134 and ischemia?

57074 ISCHEMIA?

L35 1 L34 AND ISCHEMIA?

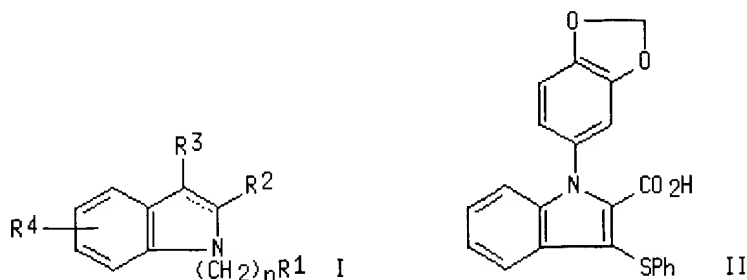
=> d 135, ibib abs fhitr, 1

L35 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text	Citing References
ACCESSION NUMBER:	1996:87548 HCAPLUS
DOCUMENT NUMBER:	124:260835
TITLE:	Indole-2-carboxylic acids as nonpeptide endothelin antagonists
INVENTOR(S):	Berryman, Kent A.; Bunker, Amy M.; Doherty, Annette M.; Edmunds, Jeremy J.
PATENT ASSIGNEE(S):	Warner-Lambert Co., USA
SOURCE:	U.S., 12 pp. CODEN: USXXAM
DOCUMENT TYPE:	Patent
LANGUAGE:	English
FAMILY ACC. NUM. COUNT:	1
PATENT INFORMATION:	

NOGEX

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5482960	A	19960109	US 1994-339381	19941114
WO 9615125	A1	19960523	WO 1995-US12672	19951002
W: CA, EE, JP, LT, LV, MX, SI				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
CA 2202051	AA	19960523	CA 1995-2202051	19951002
EP 790993	A1	19970827	EP 1995-937320	19951002
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE				
JP 10508843	T2	19980902	JP 1995-516037	19951002
PRIORITY APPLN. INFO.:			US 1994-339381	19941114
			WO 1995-US12672	19951002
OTHER SOURCE(S):		MARPAT 124:260835		
GI				



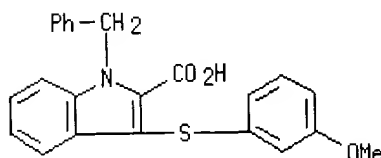
AB Novel indole and indoline nonpeptide antagonists I of endothelin I are described, wherein the dotted line indicates an optional bond; n is 0-4; R1 is Ph, in which the Ph group is substituted by methylenedioxy and further unsubstituted or substituted by, e.g., halo, C1-6 alkyl; R2 is, e.g., H, CO₂R, tetrazolyl, R = e.g., H, C1-6 alkyl,; R3 = S(O)pPh, in which p is 0, 1, or 2 and Ph is unsubstituted or substituted by, e.g., halo, NO₂, N₃; R4 is one to four independent substituents selected from, e.g., hydrogen, alkyl of 1-7 carbon atoms, alkenyl of 2-7 carbon atoms, alkynyl of 2-7 carbon atom, cycloalkyl, Ph; as well as novel intermediates used in their prepn., methods for the prepn. and pharmaceutical compns. of the same, which are useful in treating elevated levels of endothelin, essential renovascular malignant and pulmonary hypertension, cerebral infarction, cerebral **ischemia**, congestive heart failure and subarachnoid hemorrhage. Thus, e.g., phenylsulfenylation of indole-2-carboxylic acid followed by treatment with Cu(II) oxide, 4-iodo-1,2-methylenedioxybenzene, and KOH afforded 1-(benzo[1,3]dioxol-5-yl)-3-phenylsulfanyl-1H-indole-2-carboxylic acid (II). In radioligand binding assays, the following cultured cells were used: rabbit renal artery vascular smooth muscle cells (ERBA-A), Ltk-cells expressing recombinant human ETAR (HERBA-A), and CHO-K1 cells expressing recombinant human ETBR (HERBA-B); II exhibited endothelin receptor binding activity with IC₅₀ = 1.9, 3.2, and 6.5 μ M in the ERBA-A, HERBA-A, and HERBA-B assays, resp.

IT 175339-72-7P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); **THU (Therapeutic use)**; BIOL (Biological study); PREP (Preparation); USES (Uses)
(indole-2-carboxylic acids as nonpeptide endothelin antagonists)

RN 175339-72-7 HCAPLUS

RN 175339-72-7 HCAFL05
CN 1H-Indole-2-carboxylic acid, 3-[(3-methoxyphenyl)thio]-1-(phenylmethyl)-
(9CI) (CA INDEX NAME)



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(FILE 'HOME' ENTERED AT 19:21:10 ON 22 JUN 2004)

FILE 'REGISTRY' ENTERED AT 19:21:16 ON 22 JUN 2004

L1 STRUCTURE UPLOADED

L2 4 S L1

L3 579 S L1 FULL

FILE 'HCAPLUS' ENTERED AT 19:22:04 ON 22 JUN 2004

L4 39 S L3/THU
 L5 6 S L4 AND ARTHRITIS?
 L6 1 S L5 AND FAULL, A?/AU
 L7 5 S L5 NOT L6
 L8 33 S L4 NOT L5
 L9 0 S L8 AND GLOMERULAR?
 L10 0 S L8 AND LUNG () FIBROSIS?
 L11 2 S L8 AND RESTENOSIS?
 L12 0 S L11 AND FAULL, A?/AU
 L13 0 S L11 AND KETTLE, J?/AU
 L14 0 S L8 AND ALVEOLITIS?
 L15 3 S L8 AND ASTHMA?
 L16 0 S L15 AND FAULL, A?/AU
 S L1 AND KETTLE, J?/AU

FILE 'REGISTRY' ENTERED AT 19:24:50 ON 22 JUN 2004

L17 4 S L1

FILE 'HCAPLUS' ENTERED AT 19:24:51 ON 22 JUN 2004

L18 4 S L17
 L19 1 S L18 AND KETTLE, J?/AU

FILE 'HCAPLUS' ENTERED AT 19:25:00 ON 22 JUN 2004

L20 3 S L15 NOT L19
 L21 30 S L8 NOT L20
 L22 1 S L21 AND ATHEROSCLEROSIS?
 L23 0 S L22 AND FAULL, A?/AU
 L24 0 S L22 AND KETTLE, J?/AU
 L25 29 S L21 NOT L22
 L26 2 S L25 AND SKIN?
 L27 0 S L26 AND FAULL, A?/AU
 L28 3 S L25 AND KETTLE, J?/AU
 L29 0 S L26 AND KETTLE, J?/AU
 L30 27 S L25 NOT L26
 L31 0 S L30 AND MULTIPLE () SCLEROSIS?
 L32 0 S L30 AND INFLAMM? () BOWEL?
 L33 1 S L30 AND BRAIN () TRAUMA?
 L34 26 S L30 NOT L33
 L35 1 S L34 AND ISCHEMIA?

=> s l34 not l35

L36 25 L34 NOT L35

=> s l36 and myocardial? () infarction?

54476 MYOCARDIAL?

26500 INFARCTION?

16606 MYOCARDIAL? (W) INFARCTION?

L37 0 L36 AND MYOCARDIAL? (W) INFARCTION?

=> s l36 and transplant () rejection?

43773 TRANSPLANT

7027 TRANSPLANTS

46697 TRANSPLANT

(TRANSPLANT OR TRANSPLANTS)

28759 REJECTION?

7880 TRANSPLANT (W) REJECTION?

L38 0 L36 AND TRANSPLANT (W) REJECTION?

=> file caold

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	61.68	269.94

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-6.24	-11.78

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FILE COVERS 1907-1966
 FILE LAST UPDATED: 01 May 1997 (19970501/UP)

This file contains CAS Registry Numbers for easy and accurate substance identification. Title keywords, authors, patent assignees, and patent information, e.g., patent numbers, are now searchable from 1907-1966. TIFF images of CA abstracts printed between 1907-1966 are available in the PAGE display formats.

This file supports REG1stRY for direct browsing and searching of all substance data from the REGISTRY file. Enter HELP FIRST for more information.

=> d his

(FILE 'HOME' ENTERED AT 19:21:10 ON 22 JUN 2004)

FILE 'REGISTRY' ENTERED AT 19:21:16 ON 22 JUN 2004

L1 STRUCTURE UPLOADED
 L2 4 S L1
 L3 579 S L1 FULL

FILE 'HCAPLUS' ENTERED AT 19:22:04 ON 22 JUN 2004

L4 39 S L3/THU
 L5 6 S L4 AND ARTHRITIS?
 L6 1 S L5 AND FAULL, A?/AU
 L7 5 S L5 NOT L6
 L8 33 S L4 NOT L5
 L9 0 S L8 AND GLOMERULAR?
 L10 0 S L8 AND LUNG () FIBROSIS?
 L11 2 S L8 AND RESTENOSIS?
 L12 0 S L11 AND FAULL, A?/AU
 L13 0 S L11 AND KETTLE, J?/AU
 L14 0 S L8 AND ALVEOLITIS?
 L15 3 S L8 AND ASTHMA?
 L16 0 S L15 AND FAULL, A?/AU
 S L1 AND KETTLE, J?/AU

FILE 'REGISTRY' ENTERED AT 19:24:50 ON 22 JUN 2004

L17 4 S L1

FILE 'HCAPLUS' ENTERED AT 19:24:51 ON 22 JUN 2004

L18 4 S L17
 L19 1 S L18 AND KETTLE, J?/AU

FILE 'HCAPLUS' ENTERED AT 19:25:00 ON 22 JUN 2004


```

L20      3 S L15 NOT L19
L21     30 S L8  NOT L20
L22      1 S L21 AND ATHEROSCLEROSIS?
L23      0 S L22 AND FAULL, A?/AU
L24      0 S L22 AND KETTLE, J?/AU
L25     29 S L21 NOT L22
L26      2 S L25 AND SKIN?
L27      0 S L26 AND FAULL, A?/AU
L28      3 S L25 AND KETTLE, J?/AU
L29      0 S L26 AND KETTLE, J?/AU
L30     27 S L25 NOT L26
L31      0 S L30 AND MULTIPLE () SCLEROSIS?
L32      0 S L30 AND INFLAMM? () BOWEL?
L33      1 S L30 AND BRAIN () TRAUMA?
L34     26 S L30 NOT L33
L35      1 S L34 AND ISCHEMIA?
L36     25 S L34 NOT L35
L37      0 S L36 AND MYOCARDIAL? () INFARCTION?
L38      0 S L36 AND TRANSPLANT () REJECTION?

```

FILE 'CAOLD' ENTERED AT 19:29:42 ON 22 JUN 2004

=> s l3 and inflamm?

```

      7 L3
    1978 INFLAMM?
L39      0 L3 AND INFLAMM?

```

=> s l3 and arthrit?

```

      7 L3
     877 ARTHRIT?
L40      0 L3 AND ARTHRIT?

```

=> s l3 and glomerular?

```

      7 L3
     339 GLOMERULAR?
L41      0 L3 AND GLOMERULAR?

```

=> s l3 and lung () fibrosis?

```

      7 L3
    1393 LUNG
     911 LUNGS
    2281 LUNG
      (LUNG OR LUNGS)
     184 FIBROSIS?
       5 LUNG (W) FIBROSIS?
L42      0 L3 AND LUNG (W) FIBROSIS?

```

=> s l3 and restenosis?

```

      7 L3
       0 RESTENOSIS?
L43      0 L3 AND RESTENOSIS?

```

=> s l3 and asthma?

```

      7 L3
     449 ASTHMA?
L44      0 L3 AND ASTHMA?

```

=> s l3 and atherosclerosis?

```

      7 L3
    1373 ATHEROSCLEROSIS?

```

```

L45          0 L3 AND ATHEROSCLEROSIS?

=> s l3 and psoriasis?
      7 L3
      283 PSORIASIS?
L46          0 L3 AND PSORIASIS?

=> s l3 and skin?
      7 L3
      7524 SKIN?
L47          0 L3 AND SKIN?

=> s l3 and inflammatory () bowel?
      7 L3
      570 INFLAMMATORY
      74 BOWEL?
      0 INFLAMMATORY (W) BOWEL?
L48          0 L3 AND INFLAMMATORY (W) BOWEL?

=> s l3 and multiple () sclerosi?
      7 L3
      2911 MULTIPLE
      10 MULTIPLES
      2921 MULTIPLE
            (MULTIPLE OR MULTIPLES)
      346 SCLEROSI?
      171 MULTIPLE (W) SCLEROSI?
L49          0 L3 AND MULTIPLE (W) SCLEROSI?

=> s l3 and brain?
      7 L3
      7223 BRAIN?
L50          0 L3 AND BRAIN?

=> s l3 and ischemia?
      7 L3
      216 ISCHEMIA?
L51          0 L3 AND ISCHEMIA?

=> s l3 and infarction?
      7 L3
      477 INFARCTION?
L52          0 L3 AND INFARCTION?

=> s l3 and transplant () rejection?
      7 L3
      40 TRANSPLANT
      146 TRANSPLANTS
      186 TRANSPLANT
            (TRANSPLANT OR TRANSPLANTS)
      75 REJECTION?
      1 TRANSPLANT (W) REJECTION?
L53          0 L3 AND TRANSPLANT (W) REJECTION?

=> s l3 and stroke?
      7 L3
      85 STROKE?
L54          0 L3 AND STROKE?

=> file reg

```

COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	36.28	306.22
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
CA SUBSCRIBER PRICE	0.00	-11.78

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STRUCTURE FILE UPDATES: 21 JUN 2004 HIGHEST RN 697224-75-2
 DICTIONARY FILE UPDATES: 21 JUN 2004 HIGHEST RN 697224-75-2

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2004

Please note that search-term pricing does apply when
 conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more
 information enter HELP PROP at an arrow prompt in the file or refer
 to the file summary sheet on the web at:
<http://www.cas.org/ONLINE/DBSS/registryss.html>

=> d his

(FILE 'HOME' ENTERED AT 19:21:10 ON 22 JUN 2004)

FILE 'REGISTRY' ENTERED AT 19:21:16 ON 22 JUN 2004

L1 STRUCTURE UPLOADED
 L2 4 S L1
 L3 579 S L1 FULL

FILE 'HCAPLUS' ENTERED AT 19:22:04 ON 22 JUN 2004

L4 39 S L3/THU
 L5 6 S L4 AND ARTHRITIS?
 L6 1 S L5 AND FAULL, A?/AU
 L7 5 S L5 NOT L6
 L8 33 S L4 NOT L5
 L9 0 S L8 AND GLOMERULAR?
 L10 0 S L8 AND LUNG () FIBROSIS?
 L11 2 S L8 AND RESTENOSIS?
 L12 0 S L11 AND FAULL, A?/AU
 L13 0 S L11 AND KETTLE, J?/AU
 L14 0 S L8 AND ALVEOLITIS?
 L15 3 S L8 AND ASTHMA?
 L16 0 S L15 AND FAULL, A?/AU
 S L1 AND KETTLE, J?/AU

FILE 'REGISTRY' ENTERED AT 19:24:50 ON 22 JUN 2004

L17 4 S L1

FILE 'HCAPLUS' ENTERED AT 19:24:51 ON 22 JUN 2004

L18 4 S L17
 L19 1 S L18 AND KETTLE, J?/AU

FILE 'HCAPLUS' ENTERED AT 19:25:00 ON 22 JUN 2004

L20 3 S L15 NOT L19
 L21 30 S L8 NOT L20
 L22 1 S L21 AND ATHEROSCLEROSIS?
 L23 0 S L22 AND FAULL, A?/AU
 L24 0 S L22 AND KETTLE, J?/AU
 L25 29 S L21 NOT L22
 L26 2 S L25 AND SKIN?
 L27 0 S L26 AND FAULL, A?/AU
 L28 3 S L25 AND KETTLE, J?/AU
 L29 0 S L26 AND KETTLE, J?/AU
 L30 27 S L25 NOT L26
 L31 0 S L30 AND MULTIPLE () SCLEROSIS?
 L32 0 S L30 AND INFLAMM? () BOWEL?
 L33 1 S L30 AND BRAIN () TRAUMA?
 L34 26 S L30 NOT L33
 L35 1 S L34 AND ISCHEMIA?
 L36 25 S L34 NOT L35
 L37 0 S L36 AND MYOCARDIAL? () INFARCTION?
 L38 0 S L36 AND TRANSPLANT () REJECTION?

FILE 'CAOLD' ENTERED AT 19:29:42 ON 22 JUN 2004

L39 0 S L3 AND INFLAMM?
 L40 0 S L3 AND ARTHRIT?
 L41 0 S L3 AND GLOMERULAR?
 L42 0 S L3 AND LUNG () FIBROSIS?
 L43 0 S L3 AND RESTENOSIS?
 L44 0 S L3 AND ASTHMA?
 L45 0 S L3 AND ATHEROSCLEROSIS?
 L46 0 S L3 AND PSORIASIS?
 L47 0 S L3 AND SKIN?
 L48 0 S L3 AND INFLAMMATORY () BOWEL?
 L49 0 S L3 AND MULTIPLE () SCLEROSI?
 L50 0 S L3 AND BRAIN?
 L51 0 S L3 AND ISCHEMIA?
 L52 0 S L3 AND INFARCTION?
 L53 0 S L3 AND TRANSPLANT () REJECTION?
 L54 0 S L3 AND STROKE?

FILE 'REGISTRY' ENTERED AT 19:32:13 ON 22 JUN 2004

=> file hcaplus

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.42	306.64
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-11.78

FILE 'HCAPLUS' ENTERED AT 19:32:22 ON 22 JUN 2004

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FILE COVERS 1907 - 22 Jun 2004 VOL 140 ISS 26
FILE LAST UPDATED: 21 Jun 2004 (20040621/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> d his

(FILE 'HOME' ENTERED AT 19:21:10 ON 22 JUN 2004)

FILE 'REGISTRY' ENTERED AT 19:21:16 ON 22 JUN 2004

L1 STRUCTURE UPLOADED
L2 4 S L1
L3 579 S L1 FULL

FILE 'HCAPLUS' ENTERED AT 19:22:04 ON 22 JUN 2004

L4 39 S L3/THU
L5 6 S L4 AND ARTHRITIS?
L6 1 S L5 AND FAULL, A?/AU
L7 5 S L5 NOT L6
L8 33 S L4 NOT L5
L9 0 S L8 AND GLOMERULAR?
L10 0 S L8 AND LUNG () FIBROSIS?
L11 2 S L8 AND RESTENOSIS?
L12 0 S L11 AND FAULL, A?/AU
L13 0 S L11 AND KETTLE, J?/AU
L14 0 S L8 AND ALVEOLITIS?
L15 3 S L8 AND ASTHMA?
L16 0 S L15 AND FAULL, A?/AU
S L1 AND KETTLE, J?/AU

FILE 'REGISTRY' ENTERED AT 19:24:50 ON 22 JUN 2004

L17 4 S L1

FILE 'HCAPLUS' ENTERED AT 19:24:51 ON 22 JUN 2004

L18 4 S L17
L19 1 S L18 AND KETTLE, J?/AU

FILE 'HCAPLUS' ENTERED AT 19:25:00 ON 22 JUN 2004

L20 3 S L15 NOT L19
L21 30 S L8 NOT L20
L22 1 S L21 AND ATHEROSCLEROSIS?
L23 0 S L22 AND FAULL, A?/AU
L24 0 S L22 AND KETTLE, J?/AU
L25 29 S L21 NOT L22
L26 2 S L25 AND SKIN?
L27 0 S L26 AND FAULL, A?/AU
L28 3 S L25 AND KETTLE, J?/AU
L29 0 S L26 AND KETTLE, J?/AU
L30 27 S L25 NOT L26

L31 0 S L30 AND MULTIPLE () SCLEROSIS?
 L32 0 S L30 AND INFLAMM? () BOWEL?
 L33 1 S L30 AND BRAIN () TRAUMA?
 L34 26 S L30 NOT L33
 L35 1 S L34 AND ISCHEMIA?
 L36 25 S L34 NOT L35
 L37 0 S L36 AND MYOCARDIAL? () INFARCTION?
 L38 0 S L36 AND TRANSPLANT () REJECTION?

FILE 'CAOLD' ENTERED AT 19:29:42 ON 22 JUN 2004

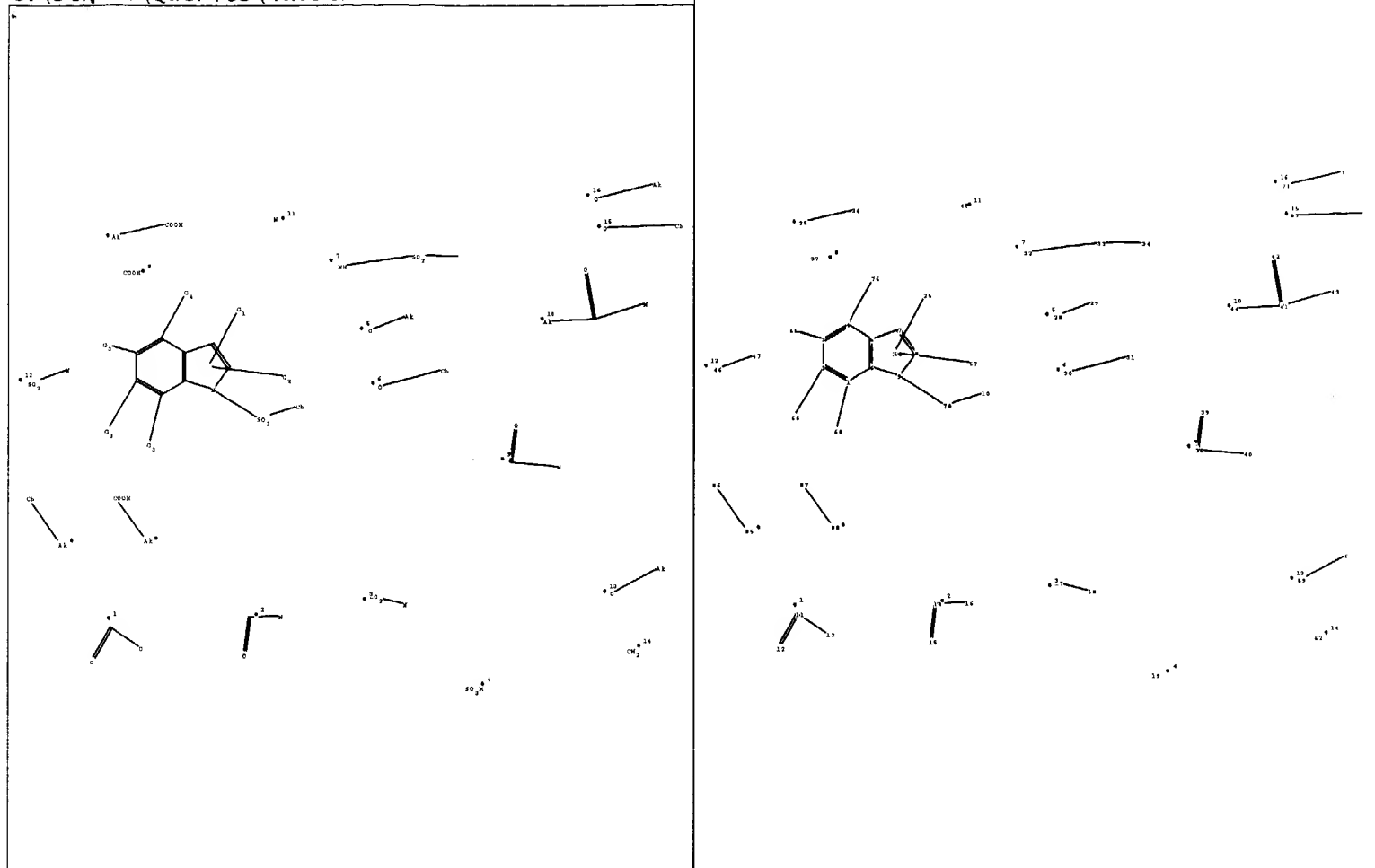
L39 0 S L3 AND INFLAMM?
 L40 0 S L3 AND ARTHRIT?
 L41 0 S L3 AND GLOMERULAR?
 L42 0 S L3 AND LUNG () FIBROSIS?
 L43 0 S L3 AND RESTENOSIS?
 L44 0 S L3 AND ASTHMA?
 L45 0 S L3 AND ATHEROSCLEROSIS?
 L46 0 S L3 AND PSORIASIS?
 L47 0 S L3 AND SKIN?
 L48 0 S L3 AND INFLAMMATORY () BOWEL?
 L49 0 S L3 AND MULTIPLE () SCLEROSI?
 L50 0 S L3 AND BRAIN?
 L51 0 S L3 AND ISCHEMIA?
 L52 0 S L3 AND INFARCTION?
 L53 0 S L3 AND TRANSPLANT () REJECTION?
 L54 0 S L3 AND STROKE?

FILE 'REGISTRY' ENTERED AT 19:32:13 ON 22 JUN 2004

FILE 'HCAPLUS' ENTERED AT 19:32:22 ON 22 JUN 2004

=> s l36 and stroke?
 22846 STROKE?
 L55 0 L36 AND STROKE?

C:\stnweb\Queries\4a.str



chain nodes :

10 11 12 13 14 15 16 17 18 19 25 28 29 30 31 32 33 35 36 37 38 39
40 41 42 43 44 45 46 47 57 59 60 62 65 66 68 69 70 71 72 76 78 85
86 87 88

ring nodes :

1 2 3 4 5 6 7 8 9

ring/chain nodes :

34

chain bonds :

1-68 2-66 3-65 4-76 9-78 10-78 11-12 11-13 14-15 14-16 17-18 28-29 30-31
32-33 33-34 35-36 38-39 38-40 41-42 41-43 41-44 46-47 59-60 69-70 71-72 85-86
87-88

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-9 7-8 8-9

exact/norm bonds :

1-68 2-66 3-65 4-76 9-78 11-12 11-13 14-15 14-16 17-18 28-29 32-33 35-36
38-39 38-40 41-42 41-43 41-44 46-47 59-60 71-72 85-86 87-88

exact bonds :

5-7 6-9 7-8 8-9 10-78 30-31 33-34 69-70

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6

isolated ring systems :

containing 1 :

G1:[*1],[*2],[*3],[*4]

G2:[*5],[*6],[*7],[*8],[*9],[*10],[*11],[*12]

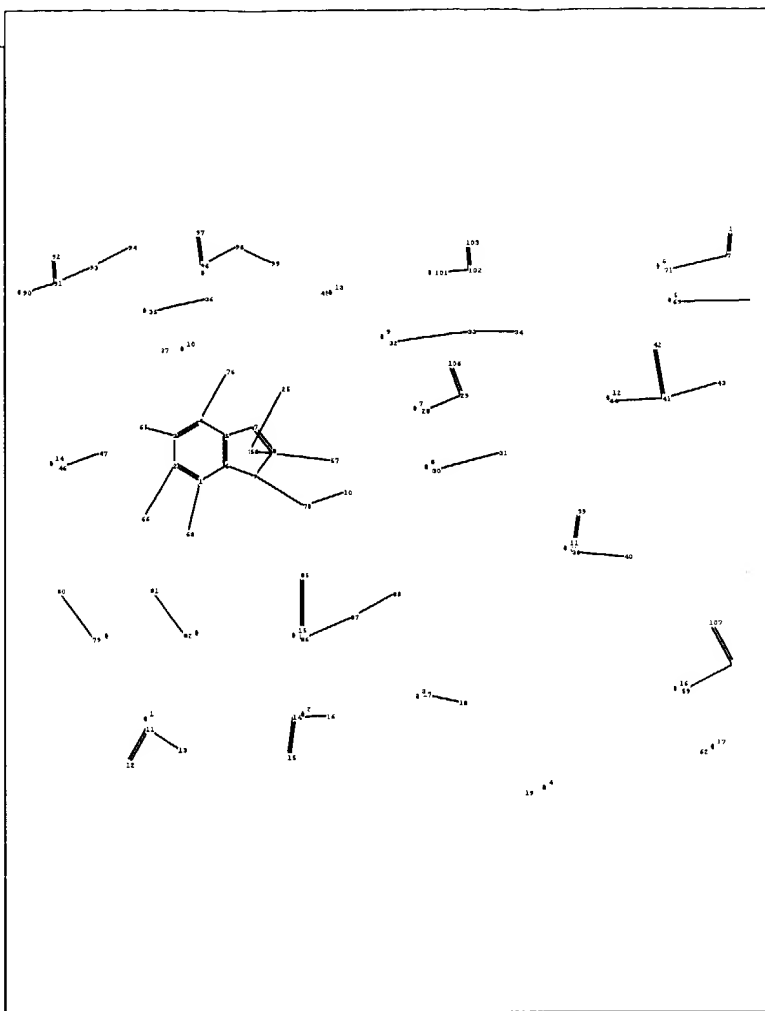
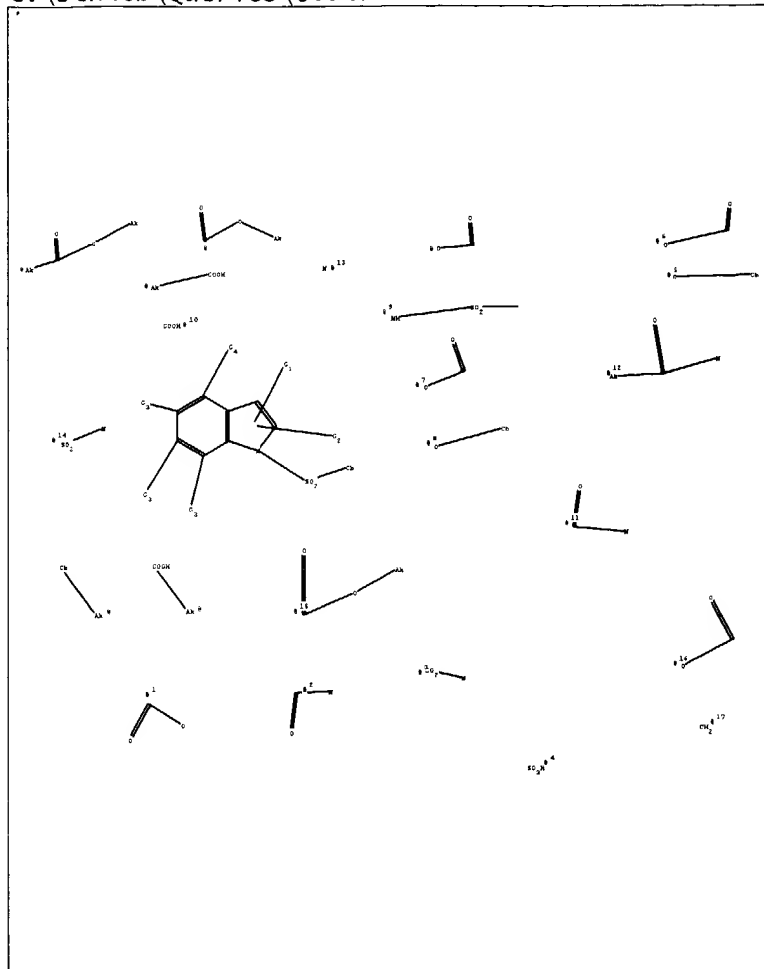
G3:H,OH,X,[*13],[*14]

G4:[*1],[*2],[*15],[*16]

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:CLASS
12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS 19:CLASS 25:CLASS
26:CLASS 28:CLASS 29:CLASS 30:CLASS 31:Atom 32:CLASS 33:CLASS 34:CLASS 35:CLASS
36:CLASS 37:CLASS 38:CLASS 39:CLASS 40:CLASS 41:CLASS 42:CLASS 43:CLASS 44:CLASS
45:CLASS 46:CLASS 47:CLASS 57:CLASS 58:CLASS 59:CLASS 60:CLASS 62:CLASS 65:CLASS
66:CLASS 68:CLASS 69:CLASS 70:Atom 71:CLASS 72:CLASS 76:CLASS 78:CLASS 85:CLASS
86:Atom 87:CLASS 88:CLASS

C:\stnweb\Queries\6.str



chain nodes :

10 11 12 13 14 15 16 17 18 19 25 28 29 30 31 32 33 35 36 37 38 39
40 41 42 43 44 45 46 47 57 59 60 62 65 66 68 69 70 71 72 76 78 79
80 81 82 85 86 87 88 90 91 92 93 94 96 97 98 99 101 102 103 105 106
107

ring nodes :

1 2 3 4 5 6 7 8 9

ring/chain nodes :

34

chain bonds :

1-68 2-66 3-65 4-76 9-78 10-78 11-12 11-13 14-15 14-16 17-18 28-29 29-106
30-31 32-33 33-34 35-36 38-39 38-40 41-42 41-43 41-44 46-47 59-60 60-107
69-70 71-72 72-105 79-80 81-82 85-86 86-87 87-88 90-91 91-92 91-93 93-94
96-97 96-98 98-99 101-102 102-103

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-9 7-8 8-9

exact/norm bonds :

1-68 2-66 3-65 4-76 9-78 11-12 11-13 14-15 14-16 17-18 28-29 29-106 32-33
35-36 38-39 38-40 41-42 41-43 41-44 46-47 59-60 60-107 71-72 72-105 79-80
81-82 85-86 86-87 87-88 90-91 91-92 91-93 93-94 96-97 96-98 98-99 101-102
102-103

exact bonds :

5-7 6-9 7-8 8-9 10-78 30-31 33-34 69-70

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6

isolated ring systems :

containing 1 :

G1:[*1],[*2],[*3],[*4],[*5],[*6]

G2:[*7],[*8],[*9],[*10],[*11],[*12],[*13],[*14],[*15]

G3:H,OH,X,[*16],[*17]

G4:[*1],[*2],[*5],[*6]

Match level :

1:Atom	2:Atom	3:Atom	4:Atom	5:Atom	6:Atom	7:Atom	8:Atom	9:Atom	10:Atom	11:CLASS
12:CLASS	13:CLASS	14:CLASS	15:CLASS	16:CLASS	17:CLASS	18:CLASS	19:CLASS	25:CLASS		
26:CLASS	28:CLASS	29:CLASS	30:CLASS	31:Atom	32:CLASS	33:CLASS	34:CLASS	35:CLASS		
36:CLASS	37:CLASS	38:CLASS	39:CLASS	40:CLASS	41:CLASS	42:CLASS	43:CLASS	44:CLASS		
45:CLASS	46:CLASS	47:CLASS	57:CLASS	58:CLASS	59:CLASS	60:CLASS	62:CLASS	65:CLASS		
66:CLASS	68:CLASS	69:CLASS	70:Atom	71:CLASS	72:CLASS	76:CLASS	78:CLASS	79:CLASS		
80:Atom	81:CLASS	82:CLASS	85:CLASS	86:CLASS	87:CLASS	88:CLASS	90:CLASS	91:CLASS		
92:CLASS	93:CLASS	94:CLASS	96:CLASS	97:CLASS	98:CLASS	99:CLASS	101:CLASS			
102:CLASS	103:CLASS	105:CLASS	106:CLASS	107:CLASS						

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 NEWS 2 "Ask CAS" for self-help around the clock
 NEWS 3 May 10 PROUSDDR now available on STN
 NEWS 4 May 19 PROUSDDR: One FREE connect hour, per account, in both May
 and June 2004
 NEWS 5 May 12 EXTEND option available in structure searching
 NEWS 6 May 12 Polymer links for the POLYLINK command completed in REGISTRY
 NEWS 7 May 17 FRFULL now available on STN
 NEWS 8 May 27 New UPM (Update Code Maximum) field for more efficient patent
 SDIs in Caplus
 NEWS 9 May 27 Caplus super roles and document types searchable in REGISTRY
 NEWS 10 May 27 Explore APOLLIT with free connect time in June 2004
 NEWS 11 Jun 22 STN Patent Forums to be held July 19-22, 2004

NEWS EXPRESS MARCH 31 CURRENT WINDOWS VERSION IS V7.00A, CURRENT
 MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP),
 AND CURRENT DISCOVER FILE IS DATED 26 APRIL 2004

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 NEWS PHONE Direct Dial and Telecommunication Network Access to STN
 NEWS WWW CAS World Wide Web Site (general information)

Enter NEWS followed by the item number or name to see news on that
 specific topic.

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* * * * * STN Columbus * * * * *

FILE 'HOME' ENTERED AT 20:15:05 ON 22 JUN 2004

=> file reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.21	0.21

FILE 'REGISTRY' ENTERED AT 20:15:12 ON 22 JUN 2004

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STRUCTURE FILE UPDATES: 21 JUN 2004 HIGHEST RN 697224-75-2
 DICTIONARY FILE UPDATES: 21 JUN 2004 HIGHEST RN 697224-75-2

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2004

Please note that search-term pricing does apply when
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Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:
<http://www.cas.org/ONLINE/DBSS/registryss.html>

=>

L1 STRUCTURE UPLOADED

=> d l1

L1 HAS NO ANSWERS

L1 STR

=> s l1

SAMPLE SEARCH INITIATED 20:17:09 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 2 TO ITERATE

100.0% PROCESSED 2 ITERATIONS

0 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS: 2 TO 124

PROJECTED ANSWERS: 0 TO 0

L2 0 SEA SSS SAM L1

=> s l1 full

THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 155.00 U.S. DOLLARS

DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y

FULL SEARCH INITIATED 20:17:14 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 5 TO ITERATE

100.0% PROCESSED 5 ITERATIONS

0 ANSWERS

SEARCH TIME: 00.00.01

L3 0 SEA SSS FUL L1

=>

L4 STRUCTURE UPLOADED

=> d l4

L4 HAS NO ANSWERS

L4 STR

=> s l4

SAMPLE SEARCH INITIATED 20:27:04 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 0 TO ITERATE

100.0% PROCESSED 0 ITERATIONS

0 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS: 0 TO 0

PROJECTED ANSWERS: 0 TO 0

L5 0 SEA SSS SAM L4

=> s l4 full

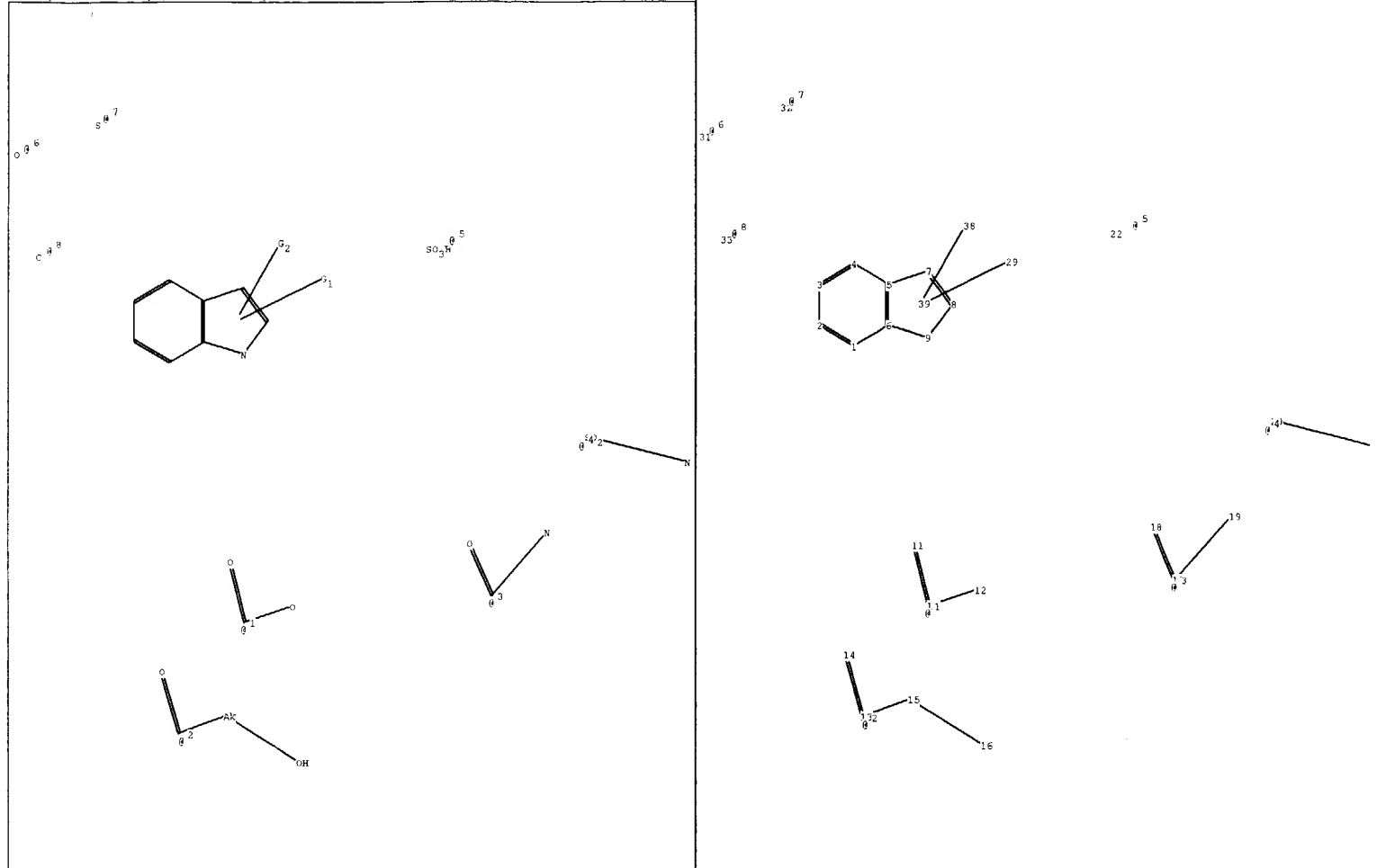
THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 155.00 U.S. DOLLARS
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y
FULL SEARCH INITIATED 20:27:08 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 1 TO ITERATE

100.0% PROCESSED 1 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.01

L6 0 SEA SSS FUL L4

=>

C:\stnweb\Queries\4.str



chain nodes :

10 11 12 13 14 15 16 17 18 19 20 21 22 29 31 32 33 38

ring nodes :

1 2 3 4 5 6 7 8 9

chain bonds :

10-12 10-11 13-14 13-15 15-16 17-18 17-19 20-21

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-9 7-8 8-9

exact/norm bonds :

6-9 8-9 10-12 10-11 13-14 13-15 15-16 17-18 17-19 20-21

exact bonds :

5-7 7-8

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6

isolated ring systems :

containing 1 :

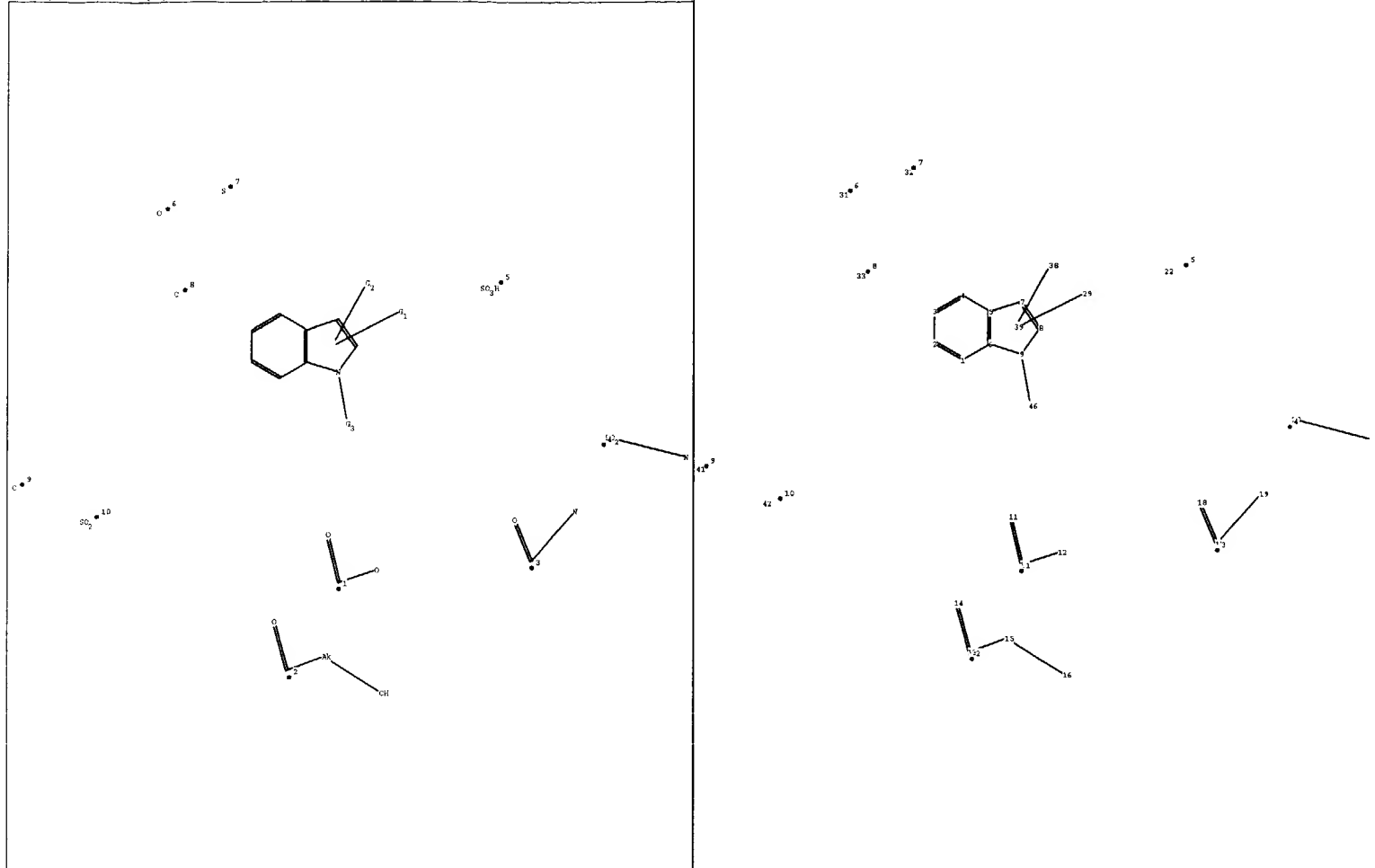
G1:CN,[*1],[*2],[*3],[*4],[*5]

G2:[*6],[*7],[*8]

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS
 11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS 19:CLASS
 20:CLASS 21:CLASS 22:CLASS 29:CLASS 30:CLASS 31:CLASS 32:CLASS 33:CLASS 38:CLASS
 39:CLASS

C:\stnweb\Queries\5.str



```

chain nodes :
  10 11 12 13 14 15 16 17 18 19 20 21 22 29 31 32 33 38 41 42 46
ring nodes :
  1 2 3 4 5 6 7 8 9
chain bonds :
  9-46 10-12 10-11 13-14 13-15 15-16 17-18 17-19 20-21
ring bonds :
  1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-9 7-8 8-9
exact/norm bonds :
  6-9 8-9 9-46 10-12 10-11 13-14 13-15 15-16 17-18 17-19 20-21
exact bonds :
  5-7 7-8
normalized bonds :
  1-2 1-6 2-3 3-4 4-5 5-6
isolated ring systems :
  containing 1 :

```

G1:CN,[*1],[*2],[*3],[*4],[*5]

G2:[*6],[*7],[*8]

G3:H,[*9],[*10]

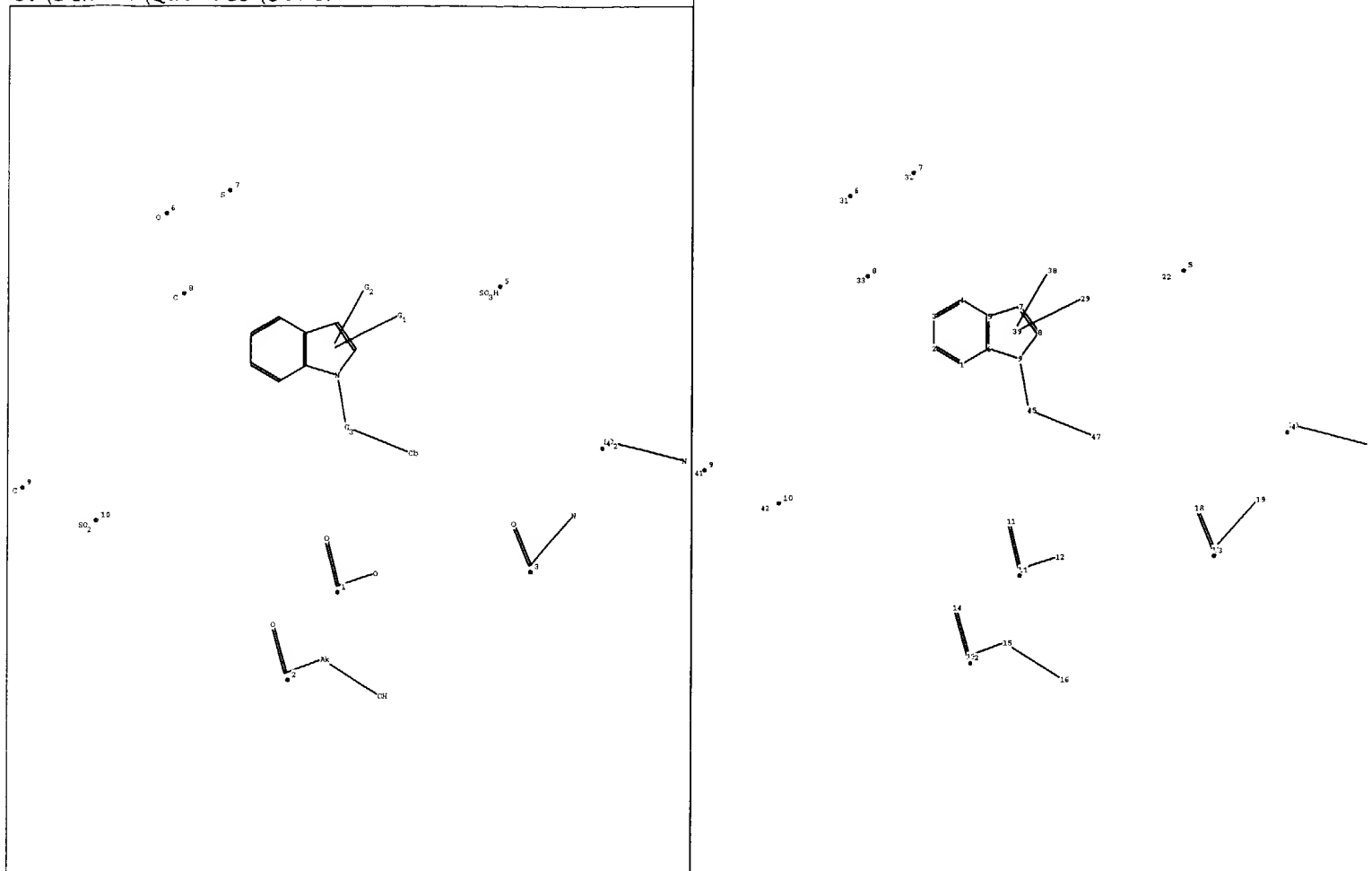
Match level :

```

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS
11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS 19:CLASS
20:CLASS 21:CLASS 22:CLASS 29:CLASS 30:CLASS 31:CLASS 32:CLASS 33:CLASS 38:CLASS
39:CLASS 41:CLASS 42:CLASS 46:CLASS

```

C:\stnweb\Queries\3.str



```

chain nodes :
  10 11 12 13 14 15 16 17 18 19 20 21 22 29 31 32 33 38 41 42 45 47
ring nodes :
  1 2 3 4 5 6 7 8 9
chain bonds :
  9-45 10-12 10-11 13-14 13-15 15-16 17-18 17-19 20-21 45-47
ring bonds :
  1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-9 7-8 8-9
exact/norm bonds :
  6-9 8-9 9-45 10-12 10-11 13-14 13-15 15-16 17-18 17-19 20-21 45-47
exact bonds :
  5-7 7-8
normalized bonds :
  1-2 1-6 2-3 3-4 4-5 5-6
isolated ring systems :
  containing 1 :

```

G1:CN,[*1],[*2],[*3],[*4],[*5]

G2:[*6],[*7],[*8]

G3:[*9],[*10]

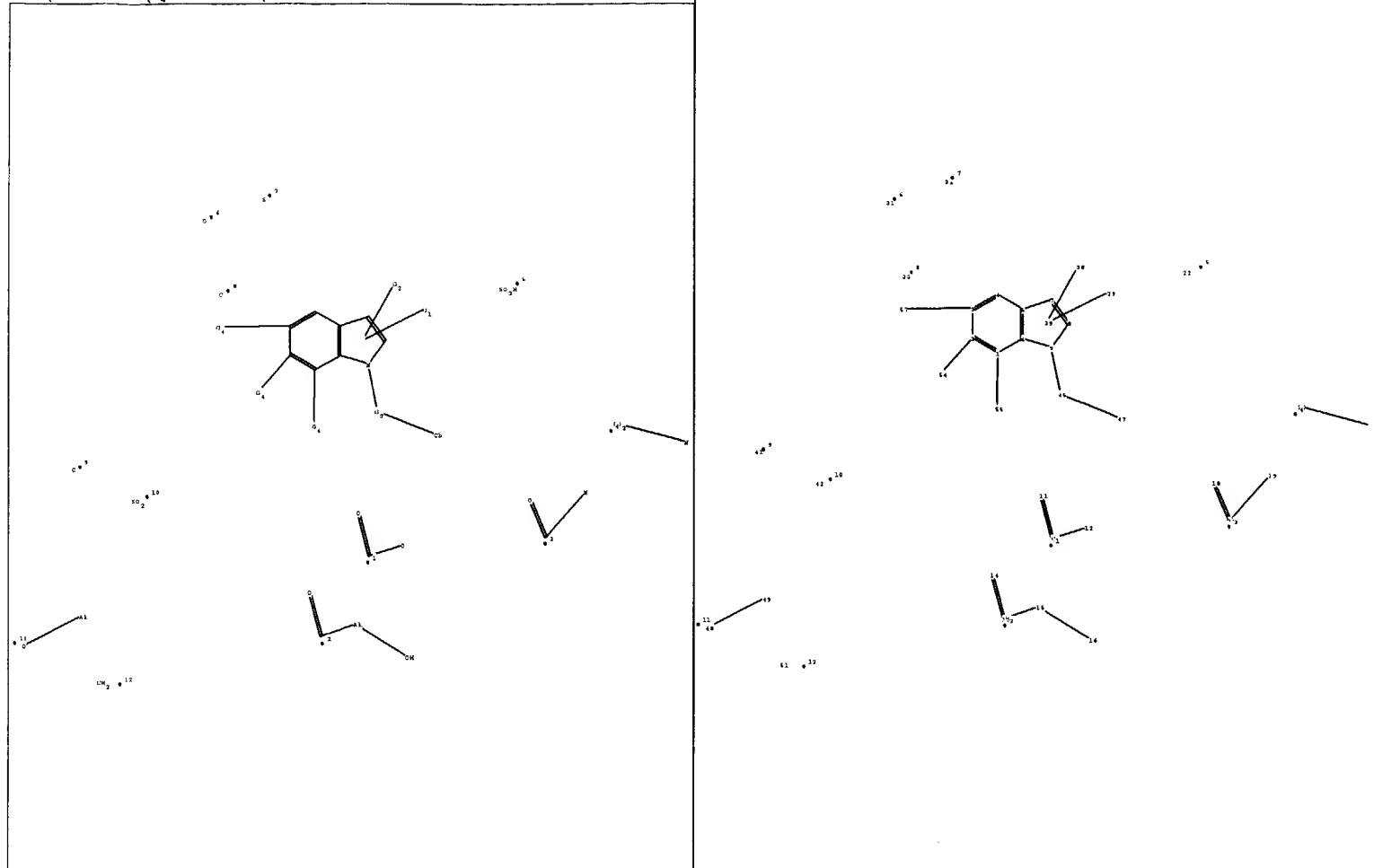
Match level :

```

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS
11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS 19:CLASS
20:CLASS 21:CLASS 22:CLASS 29:CLASS 30:CLASS 31:CLASS 32:CLASS 33:CLASS 38:CLASS
39:CLASS 41:CLASS 42:CLASS 45:CLASS 47:Atom

```


C:\stnweb\queries\4.str



```

chain nodes :
  10 11 12 13 14 15 16 17 18 19 20 21 22 29 31 32 33 38 41 42 45 47
  48 49 51 54 55 57
ring nodes :
  1 2 3 4 5 6 7 8 9
chain bonds :
  1-55 2-54 3-57 9-45 10-12 10-11 13-14 13-15 15-16 17-18 17-19 20-21 45-47
  48-49
ring bonds :
  1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-9 7-8 8-9
exact/norm bonds :
  1-55 2-54 3-57 6-9 8-9 9-45 10-12 10-11 13-14 13-15 15-16 17-18 17-19 20-21
  45-47 48-49
exact bonds :
  5-7 7-8
normalized bonds :
  1-2 1-6 2-3 3-4 4-5 5-6
isolated ring systems :
  containing 1 :

```

G1:CN,[*1],[*2],[*3],[*4],[*5]

G2:[*6],[*7],[*8]

G3:[*9],[*10]

G4:X,H,[*11],[*12]

Match level :

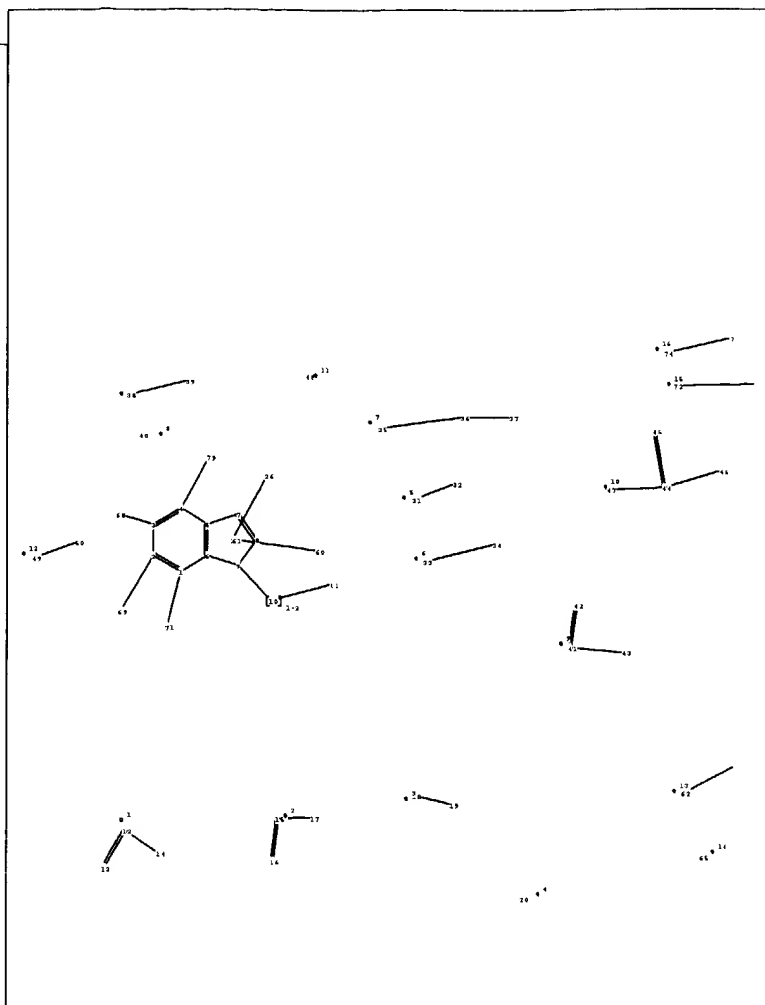
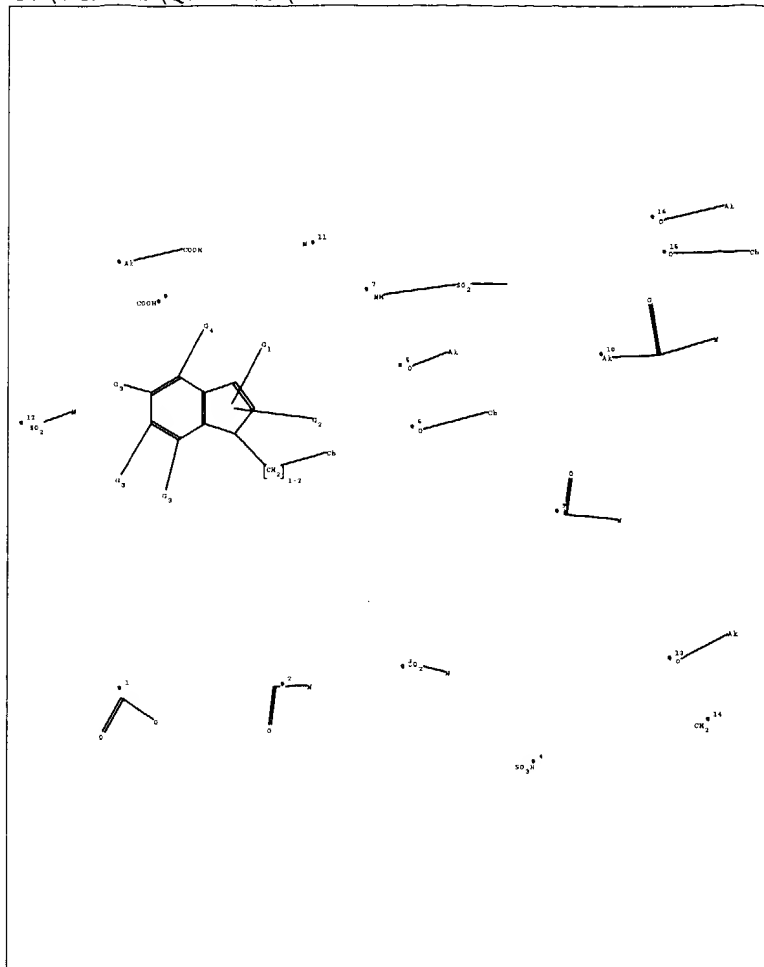
```

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS
11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS 19:CLASS
20:CLASS 21:CLASS 22:CLASS 29:CLASS 30:CLASS 31:CLASS 32:CLASS 33:CLASS 38:CLASS
39:CLASS 41:CLASS 42:CLASS 45:CLASS 47:Atom 48:CLASS 49:CLASS 51:CLASS 54:CLASS
55:CLASS

```

57:CLASS

c:\stnweb\queries\4.str



chain nodes :

10 11 12 13 14 15 16 17 18 19 20 26 31 32 33 34 35 36 38 39 40 41
42 43 44 45 46 47 48 49 50 60 62 63 65 68 69 71 72 73 74 75 79

ring nodes :

1 2 3 4 5 6 7 8 9

ring/chain nodes :

37

chain bonds :

1-71 2-69 3-68 4-79 9-10 10-11 12-13 12-14 15-16 15-17 18-19 31-32 33-34
35-36 36-37 38-39 41-42 41-43 44-45 44-46 44-47 49-50 62-63 72-73 74-75

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-9 7-8 8-9

exact/norm bonds :

1-71 2-69 3-68 4-79 12-13 12-14 15-16 15-17 18-19 31-32 35-36 38-39 41-42
41-43 44-45 44-46 44-47 49-50 62-63 74-75

exact bonds :

5-7 6-9 7-8 8-9 9-10 10-11 33-34 36-37 72-73

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6

isolated ring systems :

containing 1 :

G1:[*1],[*2],[*3],[*4]

G2:[*5],[*6],[*7],[*8],[*9],[*10],[*11],[*12]

G3:H,OH,X,[*13],[*14]

G4:[*15],[*16]

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS 11:Atom
12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS 19:CLASS 20:CLASS
26:CLASS

38:CLASS 27:CLASS 31:CLASS 32:CLASS 33:CLASS 34:Atom 35:CLASS 36:CLASS 37:CLASS
47:CLASS 39:CLASS 40:CLASS 41:CLASS 42:CLASS 43:CLASS 44:CLASS 45:CLASS 46:CLASS
68:CLASS 48:CLASS 49:CLASS 50:CLASS 60:CLASS 61:CLASS 62:CLASS 63:CLASS 65:CLASS
69:CLASS 71:CLASS 72:CLASS 73:Atom 74:CLASS 75:CLASS 79:CLASS

10	11	12	13	14	15	16	17	18	19	25	28	29	30	31	32	33	35	36	37	38	39
40	41	42	43	44	45	46	47	57	59	60	62	65	66	68	69	70	71	72	76	78	

1 2 3 4 5 6 7 8 9

34

1-68 2-66 3-65 4-76 9-78 10-78 11-12 11-13 14-15 14-16 17-18 28-29 30-31
32-33 33-34 35-36 38-39 38-40 41-42 41-43 41-44 46-47 59-60 69-70 71-72

1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-9 7-8 8-9

1-68 2-66 3-65 4-76 11-12 11-13 14-15 14-16 17-18 28-29 32-33 35-36 38-39
38-40 41-42 41-43 41-44 46-47 59-60 71-72

5-7 6-9 7-8 8-9 9-78 10-78 30-31 33-34 69-70

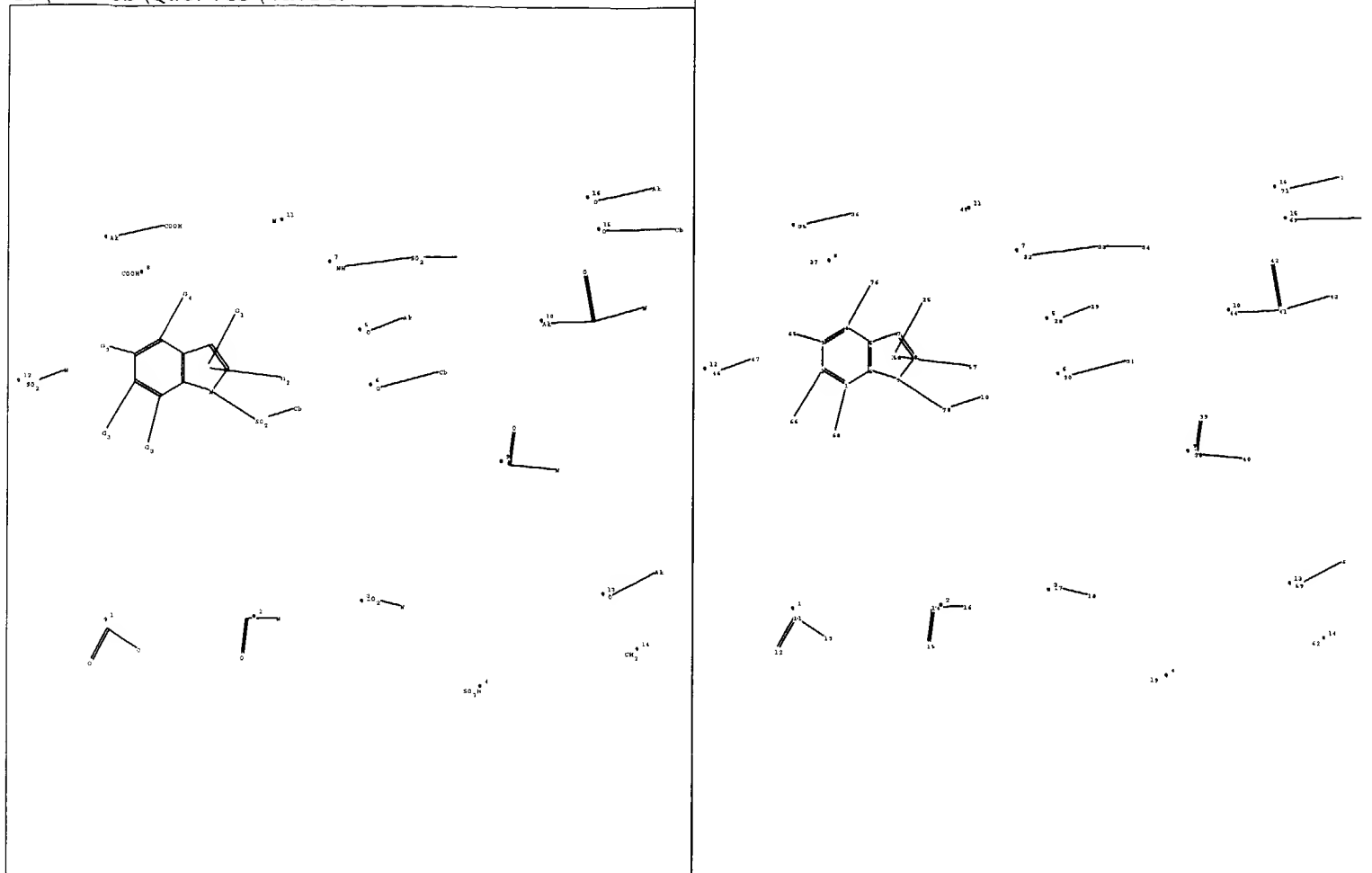
1-2 1-6 2-3 3-4 4-5 5-6

```
containing 1 :
```

G4: [*15], [*16]

```
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:CLASS
12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS 19:CLASS 25:CLASS
26:CLASS
```

	28:CLASS	29:CLASS	30:CLASS	31:Atom	32:CLASS	33:CLASS	34:CLASS	35:CLASS
36:CLASS	37:CLASS	38:CLASS	39:CLASS	40:CLASS	41:CLASS	42:CLASS	43:CLASS	44:CLASS
45:CLASS	46:CLASS	47:CLASS	57:CLASS	58:CLASS	59:CLASS	60:CLASS	62:CLASS	65:CLASS
66:CLASS	68:CLASS	69:CLASS	70:Atom	71:CLASS	72:CLASS	76:CLASS	78:CLASS	



chain nodes :

10 11 12 13 14 15 16 17 18 19 25 28 29 30 31 32 33 35 36 37 38 39
40 41 42 43 44 45 46 47 57 59 60 62 65 66 68 69 70 71 72 76 78

ring nodes :

1 2 3 4 5 6 7 8 9

ring/chain nodes :

34

chain bonds :

1-68 2-66 3-65 4-76 9-78 10-78 11-12 11-13 14-15 14-16 17-18 28-29 30-31
32-33 33-34 35-36 38-39 38-40 41-42 41-43 41-44 46-47 59-60 69-70 71-72

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-9 7-8 8-9

exact/norm bonds :

1-68 2-66 3-65 4-76 9-78 11-12 11-13 14-15 14-16 17-18 28-29 32-33 35-36
38-39 38-40 41-42 41-43 41-44 46-47 59-60 71-72

exact bonds :

5-7 6-9 7-8 8-9 10-78 30-31 33-34 69-70

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6

isolated ring systems :

containing 1 :

G1:[*1],[*2],[*3],[*4]

G2:[*5],[*6],[*7],[*8],[*9],[*10],[*11],[*12]

G3:H,OH,X,[*13],[*14]

G4:[*15],[*16]

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:CLASS
12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS 19:CLASS 25:CLASS
26:CLASS

	28:CLASS	29:CLASS	30:CLASS	31:Atom	32:CLASS	33:CLASS	34:CLASS	35:CLASS
36:CLASS	37:CLASS	38:CLASS	39:CLASS	40:CLASS	41:CLASS	42:CLASS	43:CLASS	44:CLASS
45:CLASS	46:CLASS	47:CLASS	57:CLASS	58:CLASS	59:CLASS	60:CLASS	62:CLASS	65:CLASS
66:CLASS	68:CLASS	69:CLASS	70:Atom	71:CLASS	72:CLASS	76:CLASS	78:CLASS	

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 and June 2004
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 SDIs in Caplus
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 MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP),
 AND CURRENT DISCOVER FILE IS DATED 26 APRIL 2004
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* * * * * STN Columbus * * * * *

FILE 'HOME' ENTERED AT 18:53:03 ON 22 JUN 2004

=>

THIS COMMAND NOT AVAILABLE IN THE CURRENT FILE
 Some commands only work in certain files. For example, the EXPAND
 command can only be used to look at the index in a file which has an
 index. Enter "HELP COMMANDS" at an arrow prompt (=>) for a list of
 commands which can be used in this file.

=> file reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.21	0.21

FILE 'REGISTRY' ENTERED AT 18:53:19 ON 22 JUN 2004
 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
 PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
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Property values tagged with IC are from the ZIC/VINITI data file
 provided by InfoChem.

STRUCTURE FILE UPDATES: 21 JUN 2004 HIGHEST RN 697224-75-2
 DICTIONARY FILE UPDATES: 21 JUN 2004 HIGHEST RN 697224-75-2

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2004

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:
<http://www.cas.org/ONLINE/DBSS/registryss.html>

=>

L1 STRUCTURE UPLOADED

=> d l1

L1 HAS NO ANSWERS

L1 STR

=> s l1

SAMPLE SEARCH INITIATED 18:53:34 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 18 TO ITERATE

100.0% PROCESSED 18 ITERATIONS

0 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS: 106 TO 614

PROJECTED ANSWERS: 0 TO 0

L2 0 SEA SSS SAM L1

=> s l1 full

THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 155.00 U.S. DOLLARS

DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y

FULL SEARCH INITIATED 18:53:39 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 455 TO ITERATE

100.0% PROCESSED 455 ITERATIONS

0 ANSWERS

SEARCH TIME: 00.00.01

L3 0 SEA SSS FUL L1

=>

L4 STRUCTURE UPLOADED

=> d l4

L4 HAS NO ANSWERS

L4 STR

=> s l4

SAMPLE SEARCH INITIATED 18:55:11 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 23 TO ITERATE

100.0% PROCESSED 23 ITERATIONS

0 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**
 PROJECTED ITERATIONS: 173 TO 747
 PROJECTED ANSWERS: 0 TO 0

L5 0 SEA SSS SAM L4

=> s 14 full

THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 155.00 U.S. DOLLARS
 DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y
 FULL SEARCH INITIATED 18:55:16 FILE 'REGISTRY'
 FULL SCREEN SEARCH COMPLETED - 527 TO ITERATE

100.0% PROCESSED 527 ITERATIONS 0 ANSWERS
 SEARCH TIME: 00.00.01

L6 0 SEA SSS FUL L4

=>

L7 STRUCTURE UPLOADED

=> 17

L7 IS NOT A RECOGNIZED COMMAND

The previous command name entered was not recognized by the system.
 For a list of commands available to you in the current file, enter
 "HELP COMMANDS" at an arrow prompt (=>).

=> d 17

L7 HAS NO ANSWERS

L7 STR

=> s 17

SAMPLE SEARCH INITIATED 18:56:19 FILE 'REGISTRY'
 SAMPLE SCREEN SEARCH COMPLETED - 0 TO ITERATE

100.0% PROCESSED 0 ITERATIONS 0 ANSWERS
 SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS: 0 TO 0

PROJECTED ANSWERS: 0 TO 0

L8 0 SEA SSS SAM L7

=> s 17 full

THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 155.00 U.S. DOLLARS
 DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y
 FULL SEARCH INITIATED 18:56:26 FILE 'REGISTRY'
 FULL SCREEN SEARCH COMPLETED - 10 TO ITERATE

100.0% PROCESSED 10 ITERATIONS 0 ANSWERS
 SEARCH TIME: 00.00.01

L9 0 SEA SSS FUL L7

=>